wwPDB EM Validation Summary Report (i)

Oct 14, 2021 – 10:51 pm BST

PDB ID	:	7PJW
EMDB ID	:	EMD-13462
Title	:	Structure of the 70S-EF-G-GDP-Pi ribosome complex with tRNAs in hybrid state 2 (H2-EF-G-GDP-Pi)
Authors	:	Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on	:	2021-08-24
Resolution	:	4.00 Å(reported)
Based on initial models	:	5LZD, 5J9Z, 4AQY, 6YSS

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

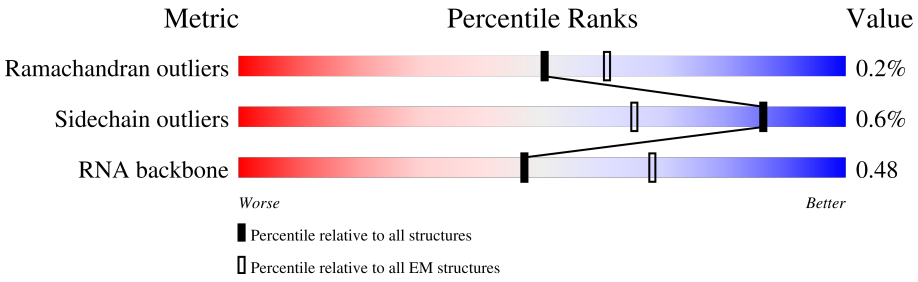
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	57	77% 98%
2	1	55	73% 91% 9%
3	2	46	65% 100%
4	3	65	77% 98%
5	4	38	66% 100%
6	5	165	79% 79% 21%
7	6	70	94% 79% 16% 6%
8	A	2903	29% 73% 26%

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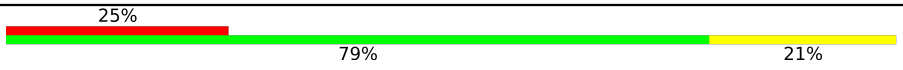
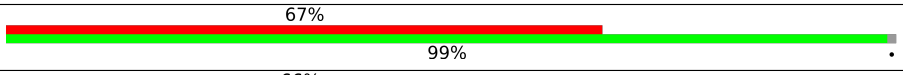
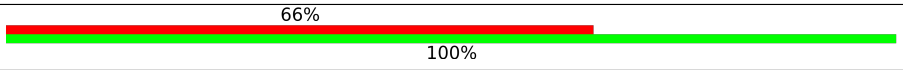
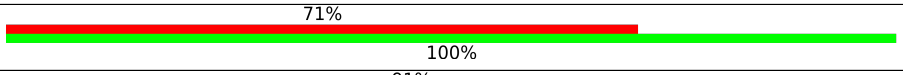
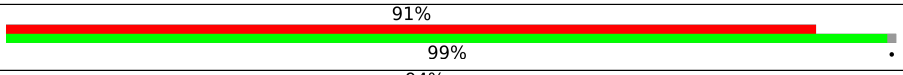
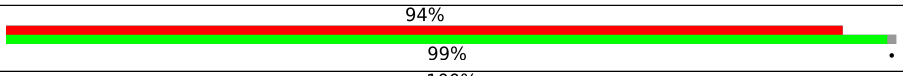
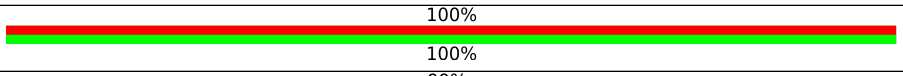
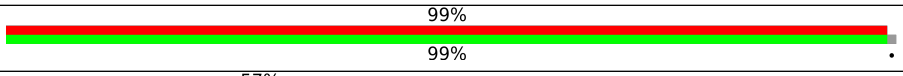
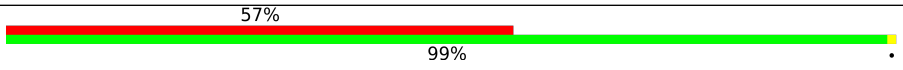
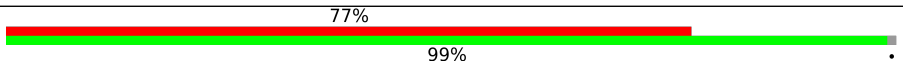
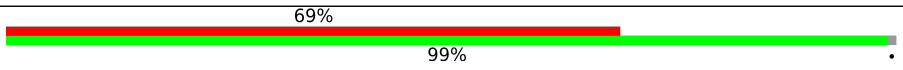
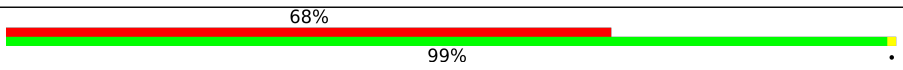
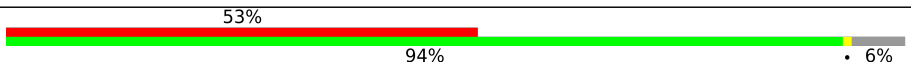
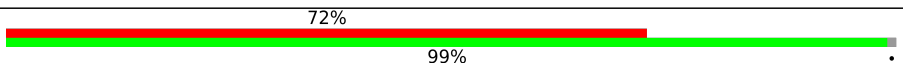
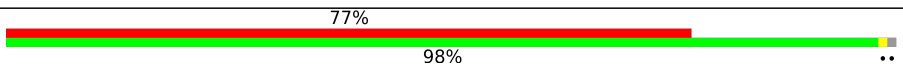
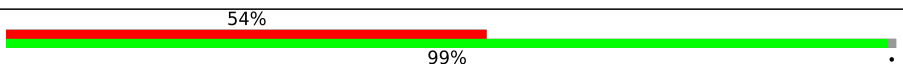
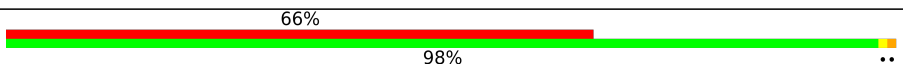
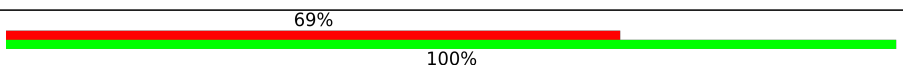
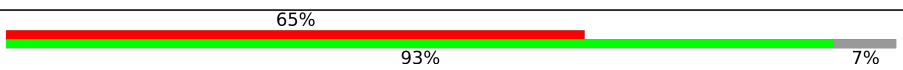
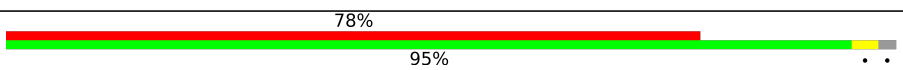
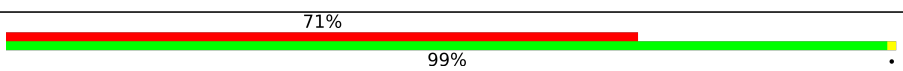
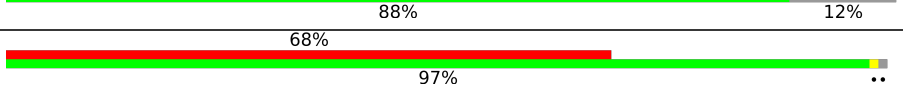
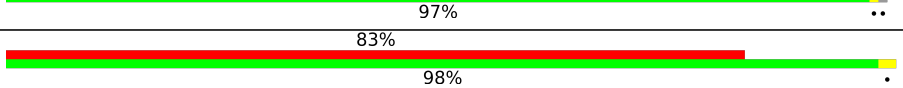
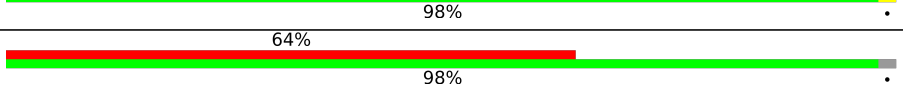
Mol	Chain	Length	Quality of chain
9	B	120	
10	C	273	
11	D	209	
12	E	201	
13	F	179	
14	G	177	
15	H	149	
16	I	142	
17	J	142	
18	K	123	
19	L	144	
20	M	136	
21	N	127	
22	O	117	
23	P	115	
24	Q	118	
25	R	103	
26	S	110	
27	T	100	
28	U	104	
29	V	94	
30	W	85	
31	X	78	
32	Y	63	
33	Z	59	

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Mol	Chain	Length	Quality of chain
34	a	1542	49% 76% 23%
35	b	240	90% 90% 9%
36	c	233	83% 88% 12%
37	d	206	92% 100%
38	e	167	83% 94% 6%
39	f	135	72% 74% 26%
40	g	179	84% 84% 16%
41	h	130	82% 99%
42	i	130	92% 97%
43	j	103	90% 94% 5%
44	k	129	77% 89% 10%
45	l	124	83% 98%
46	m	118	96% 96%
47	n	102	91% 99%
48	o	89	78% 99%
49	p	82	74% 99%
50	q	84	75% 95% 5%
51	r	75	81% 87% 13%
52	s	92	89% 89% 11%
53	t	87	91% 98%
54	u	71	92% 90% 8%
55	v	77	94% 68% 30%
56	w	76	97% 50% 38% 12%
57	x	704	98% 98%
58	y	2	100% 50% 50%

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Mol	Chain	Length	Quality of chain
59	z	33	21% 15% 15% 67%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 152719 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	5	131	647	385	131	131	0	0

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62339	27816	11471	20149	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 12 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	I	141	Total	C	N	O	0	0
			693	411	141	141		

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 29 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total 575	C 356	N 116	O 102	S 1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total 509	C 313	N 99	O 95	S 2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	58	Total 449	C 281	N 87	O 79	S 2	0	0

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total 33050	C 14748	N 6057	O 10705	P 1540	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	703	Total	C	N	O	S	0	0
			5444	3429	942	1048	25		

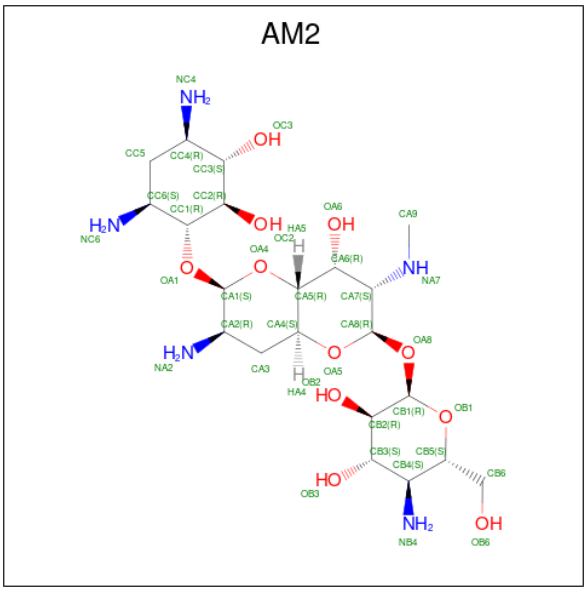
- Molecule 58 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 59 is a RNA chain called mRNA.

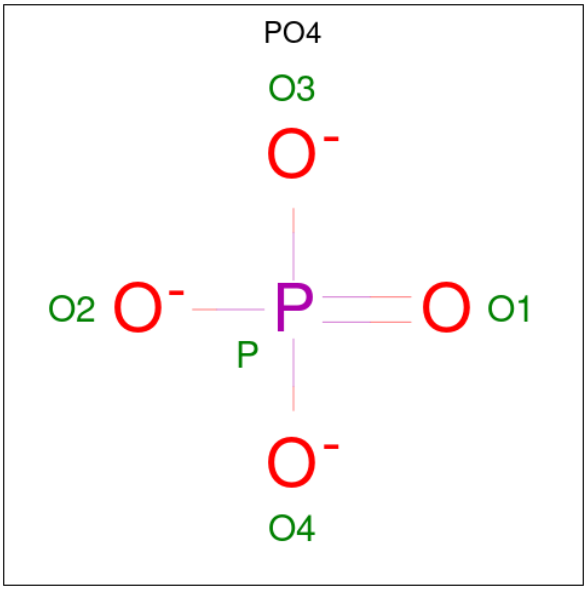
Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 60 is APRAMYCIN (three-letter code: AM2) (formula: $C_{21}H_{41}N_5O_{11}$).



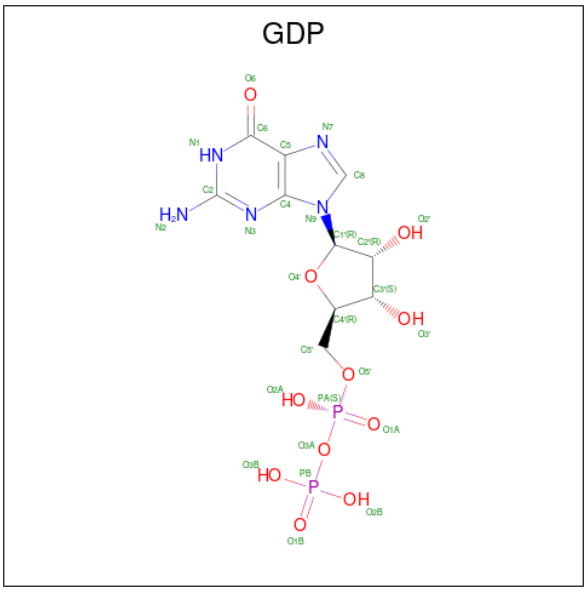
Mol	Chain	Residues	Atoms				AltConf
60	a	1	Total	C	N	O	0
			37	21	5	11	

- Molecule 61 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
61	x	1	Total	O	P	0
			5	4	1	

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



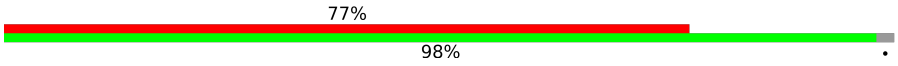
Mol	Chain	Residues	Atoms					AltConf
62	x	1	Total	C	N	O	P	0
			28	10	5	11	2	

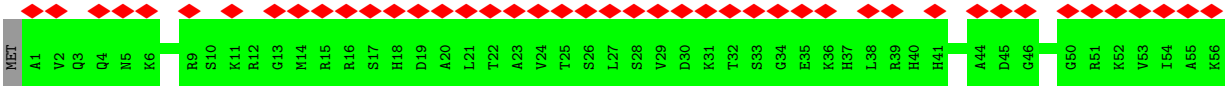
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 50S ribosomal protein L32

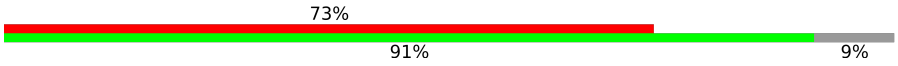
Chain 0:

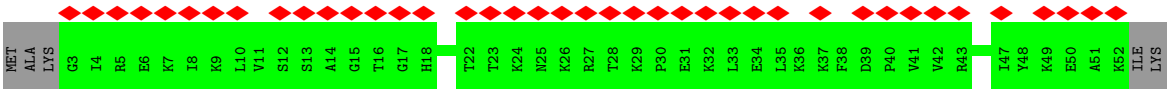




• Molecule 2: 50S ribosomal protein L33

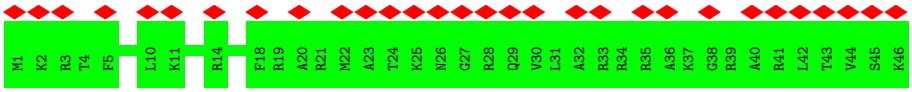
Chain 1:





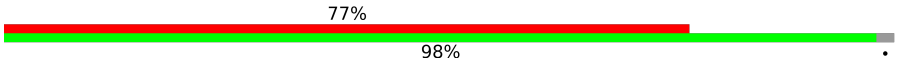
• Molecule 3: 50S ribosomal protein L34

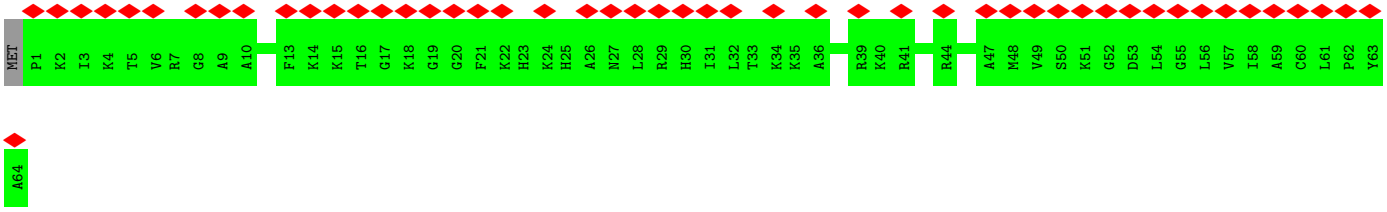
Chain 2:



• Molecule 4: 50S ribosomal protein L35

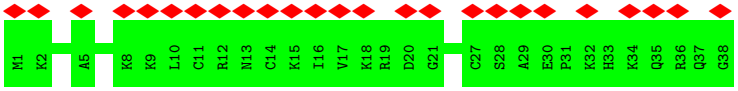
Chain 3:





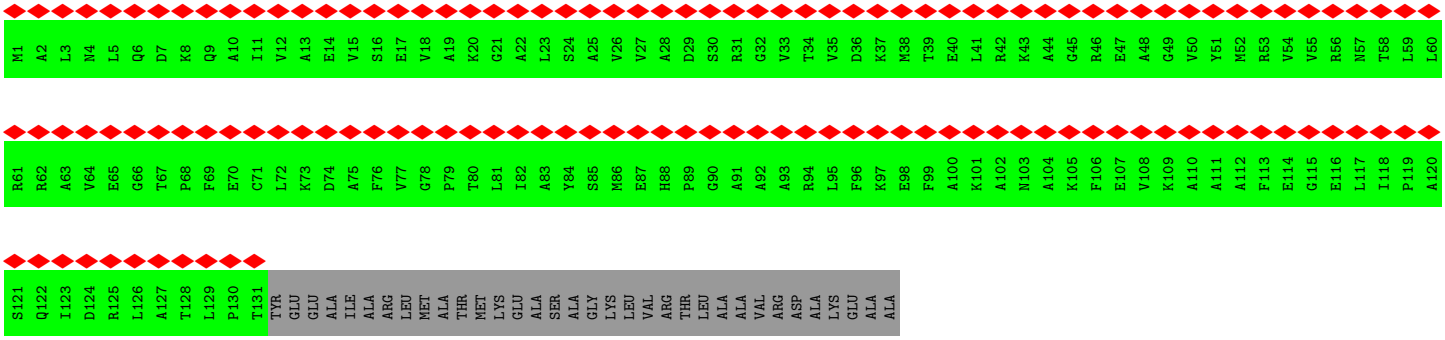
• Molecule 5: 50S ribosomal protein L36

Chain 4:



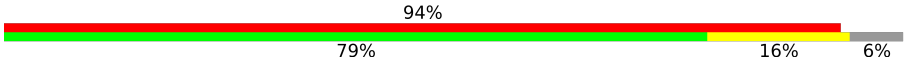
• Molecule 6: 50S ribosomal protein L10

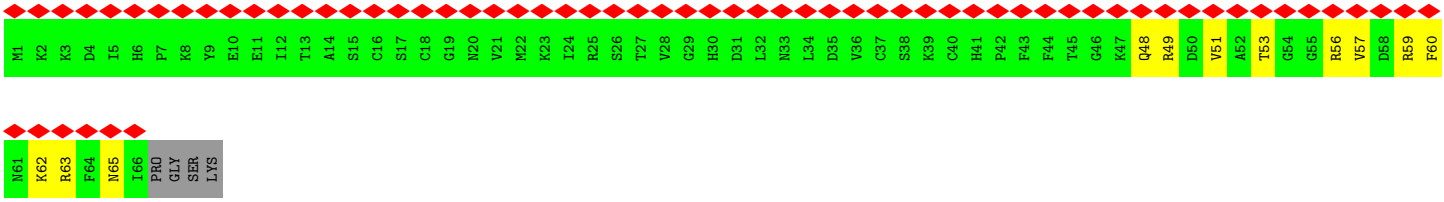
Chain 5:



• Molecule 7: 50S ribosomal protein L31

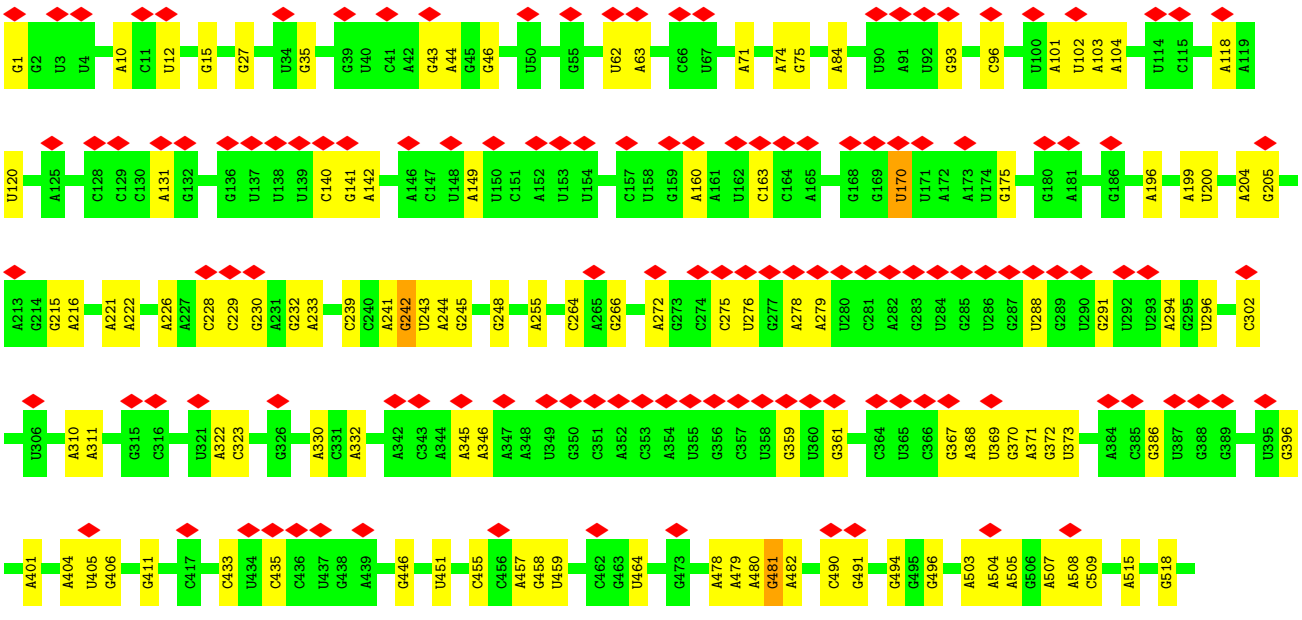
Chain 6:

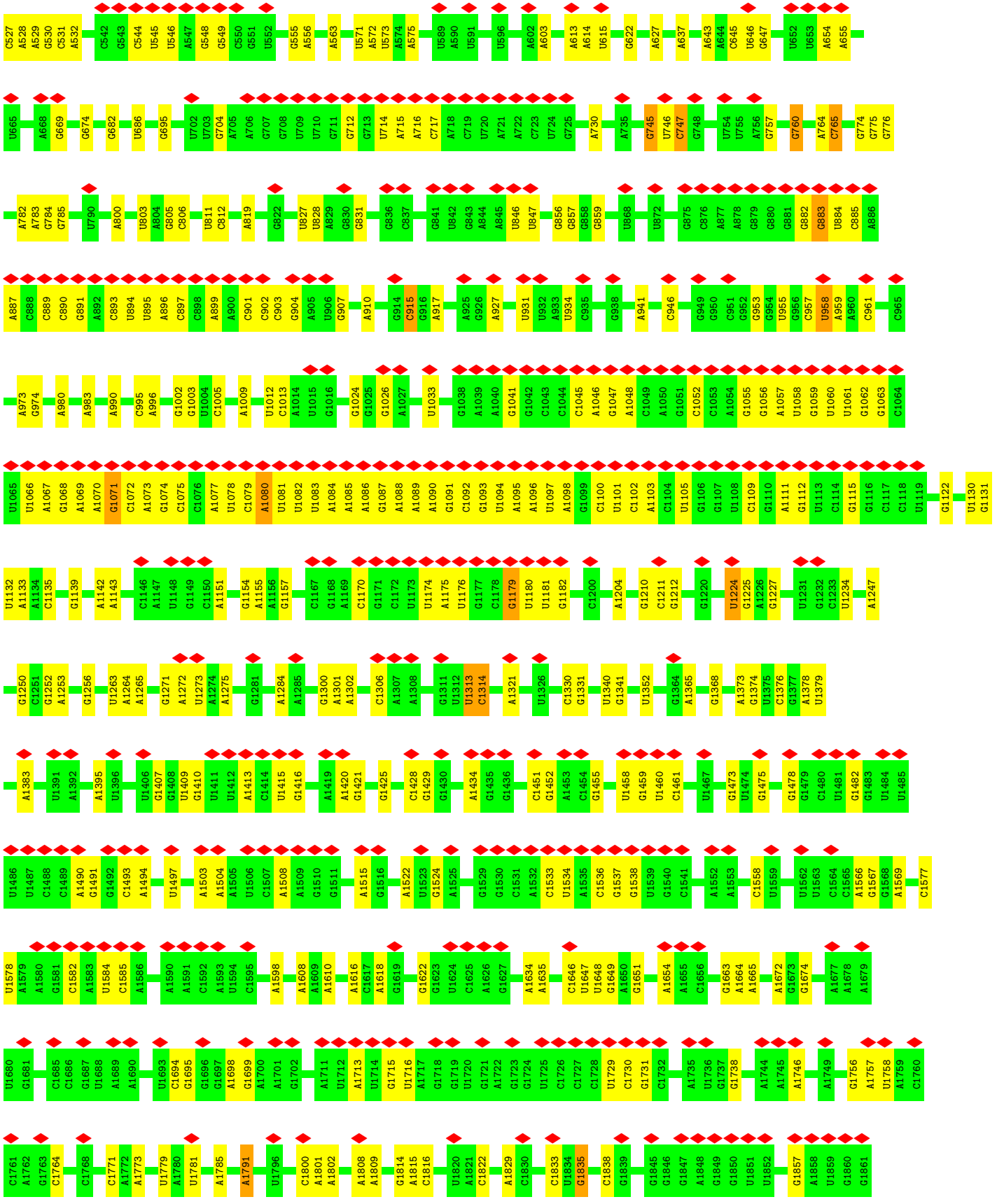


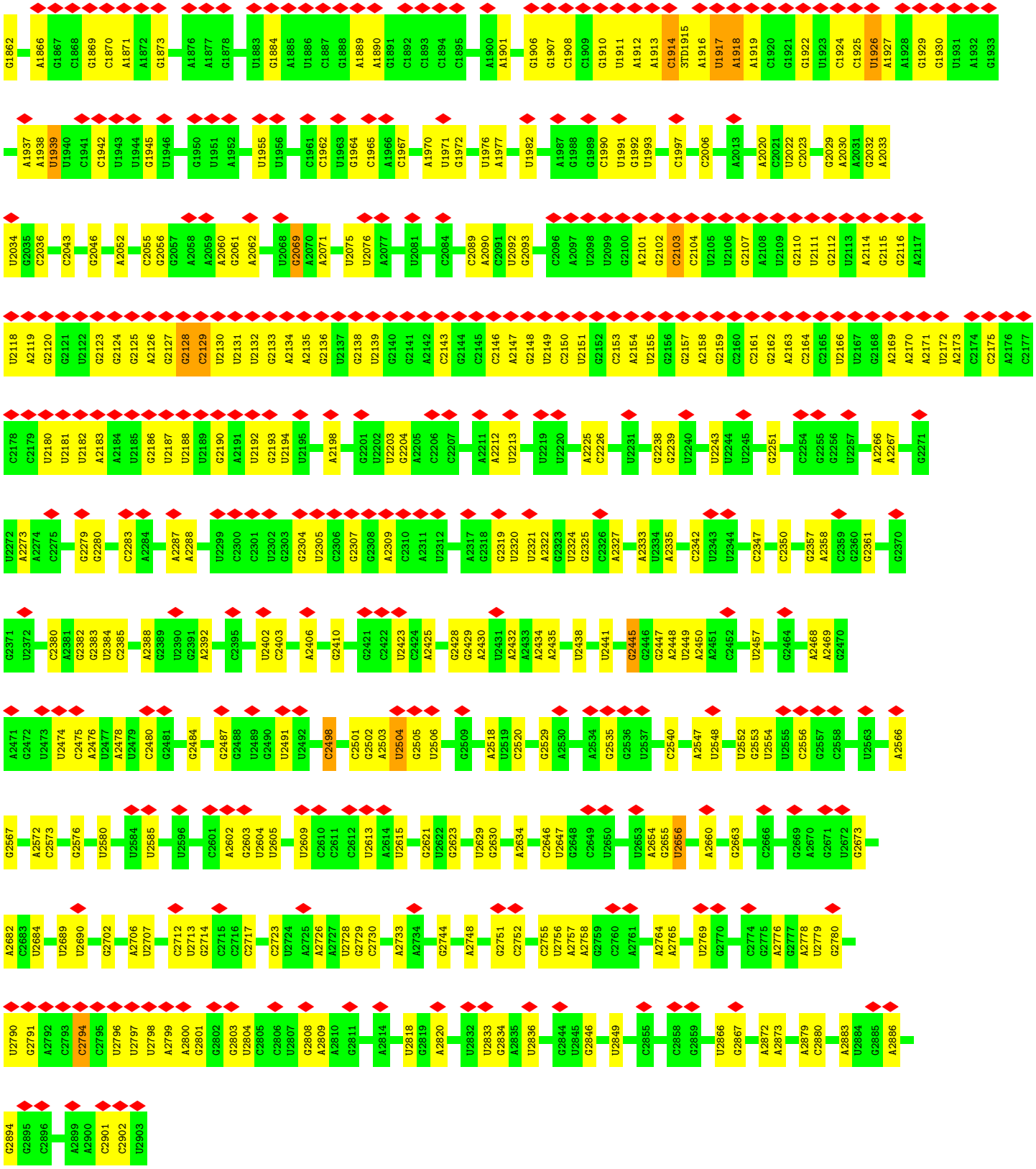


• Molecule 8: 23S ribosomal RNA

Chain A:

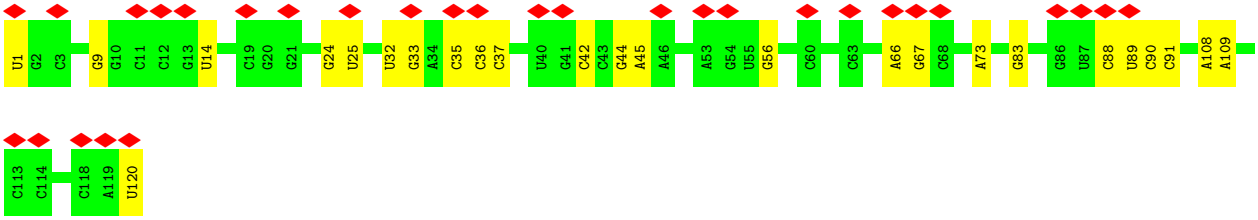



C527 A528 A529 G530 C531 A532 C542 G543 C544 U545 U546 A547 G548 G549 C550 G551 U552 G555 A556 A563 U571 A572 U573 A574 A575 U589 A590 U591 U596 A602 A603 A613 A614 U615 G622 A627 A637 A643 A644 C645 U646 G647 U652 U653 A654 A655
U665 A668 G669 G674 G682 U686 G695 U702 U703 G704 A705 A706 G707 G708 U709 U710 G711 G712 G713 U714 A715 A716 C717 A718 C719 U720 A721 A722 C723 U724 G725 A730 A735 G745 U746 C747 G748 U754 U755 A756 G757 G760 A764 C765 G774 G775 G776
A782 A783 G784 G785 U790 A800 U803 A804 G805 C806 U811 C812 A819 G822 U827 U828 A829 G830 G831 G836 C837 G841 U842 G843 A844 A845 U846 U847 G856 G857 G858 G859 U868 U872 G875 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A886
A887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 C903 G904 A905 U906 G907 A910 G914 C915 G916 A917 A925 G926 A927 U931 U932 A933 U934 C935 G938 A941 C946 G949 G950 C951 G952 G953 G954 U955 G956 C957 U958 A959 A960 C961 C965
A973 G974 A980 A983 A990 C995 A996 G1002 G1003 U1004 C1005 A1009 U1012 C1013 A1014 U1015 G1016 G1024 G1025 G1026 A1027 U1033 G1038 A1039 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064
U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 C1110 A1111 G1112 U1113 C1114 G1115 G1116 C1117 C1118 U1119 G1122 U1130 G1131
U1132 A1133 A1134 C1135 G1139 A1142 A1143 C1146 A1147 U1148 G1149 C1150 A1151 G1154 A1155 A1156 G1157 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 C1200 A1204 G1210 C1211 G1212 G1220 U1224 G1225 A1226 G1227 U1231 G1232 C1233 U1234 A1247
G1250 C1251 G1252 A1253 G1256 U1263 A1264 A1265 G1271 A1272 U1273 A1274 A1275 G1281 A1284 A1285 G1300 A1301 A1302 C1306 A1307 A1308 G1311 U1312 U1313 C1314 A1321 U1326 C1330 G1331 U1340 G1341 U1352 G1364 A1365 G1368 A1373 G1374 U1375 C1376 G1377 A1378 U1379
A1383 U1391 A1392 A1395 U1396 U1406 G1407 G1408 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 A1419 A1420 G1421 G1425 C1428 G1429 G1430 A1434 G1435 G1436 C1451 G1452 A1453 C1454 G1455 U1458 G1459 U1460 C1461 U1467 G1473 U1474 G1475 G1478 G1479 C1480 U1481 G1482 G1483 U1484 U1485
U1486 U1487 C1488 C1489 A1490 G1491 G1492 C1493 A1494 U1497 A1503 A1504 A1505 U1506 C1507 A1508 A1509 G1510 G1511 A1515 G1516 A1522 U1523 G1524 A1525 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 A1552 A1553 C1558 U1559 U1562 U1563 C1564 C1565 A1566 G1567 G1568 A1569 C1577
U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 A1590 A1591 C1592 A1593 U1594 C1595 A1598 A1608 A1609 A1610 A1616 C1617 A1618 G1619 G1622 G1623 U1624 C1625 A1626 G1627 A1634 A1635 C1646 U1647 U1648 G1649 A1650 G1651 A1654 A1655 C1656 G1663 A1664 A1665 A1672 G1673 G1674 A1677 A1678 A1679
U1680 G1681 C1685 C1686 G1687 U1688 A1689 A1690 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1702 A1711 U1712 A1713 U1714 G1715 U1716 A1717 G1718 G1719 U1720 G1721 A1722 G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 A1735 U1736 G1737 G1738 A1744 A1745 A1746 A1749 G1756 A1757 U1758 A1759 C1760
C1761 A1762 G1763 C1764 C1768 C1771 A1772 A1773 U1779 A1780 U1781 A1785 A1791 U1796 C1800 A1801 A1802 A1808 A1809 G1814 A1815 C1816 U1820 A1821 C1822 A1829 C1830 C1833 U1834 G1835 C1838 G1839 G1845 G1846 G1847 A1848 G1849 G1850 U1851 U1852 G1857 A1858 U1859 G1860 G1861



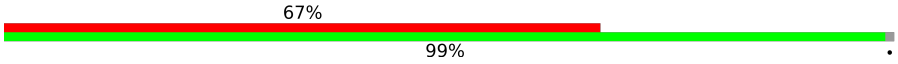
• Molecule 9: 5S ribosomal RNA

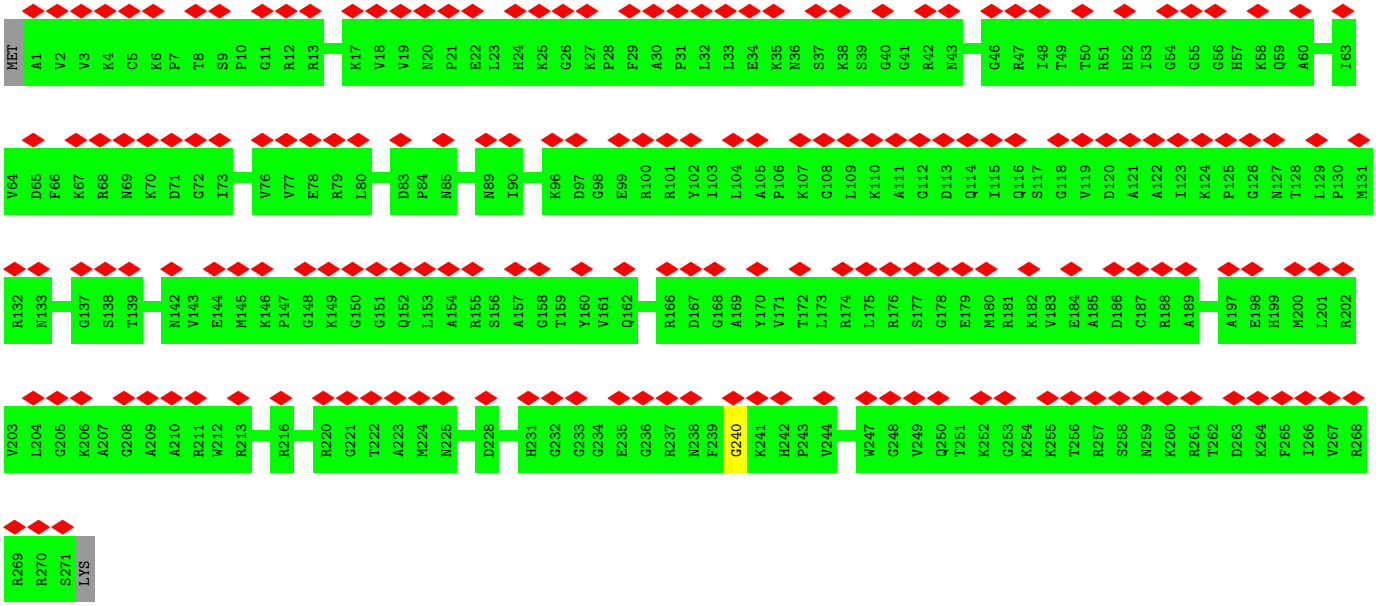
Chain B:



• Molecule 10: 50S ribosomal protein L2

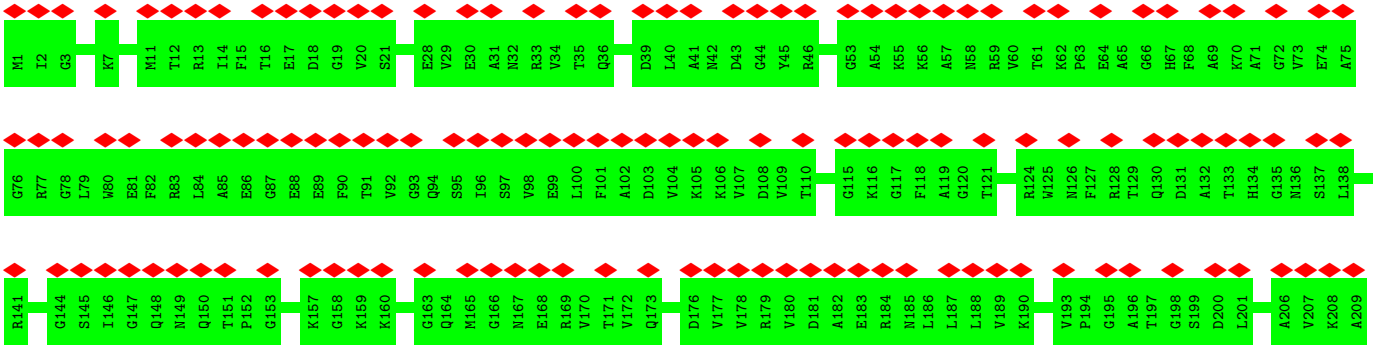
Chain C:





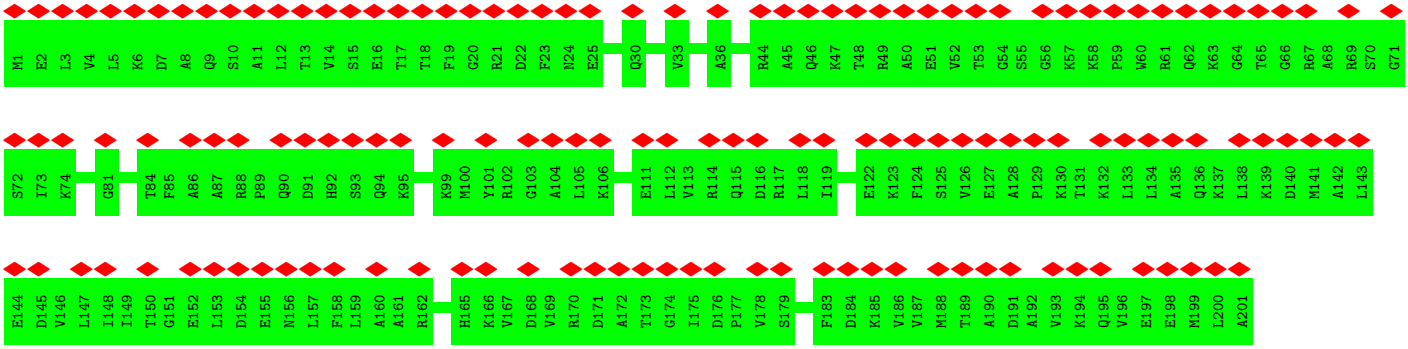
• Molecule 11: 50S ribosomal protein L3

Chain D:



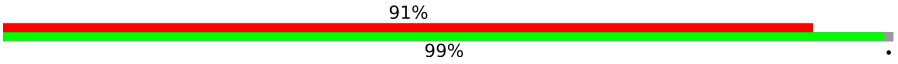
• Molecule 12: 50S ribosomal protein L4

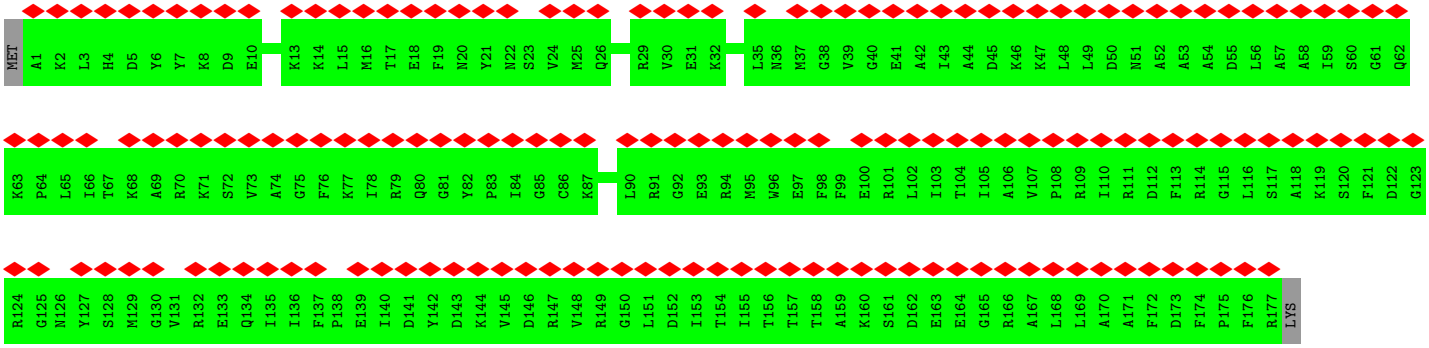
Chain E:



• Molecule 13: 50S ribosomal protein L5

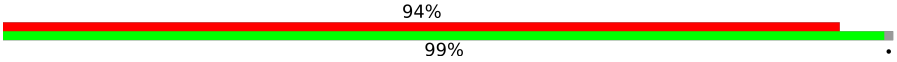
Chain F:

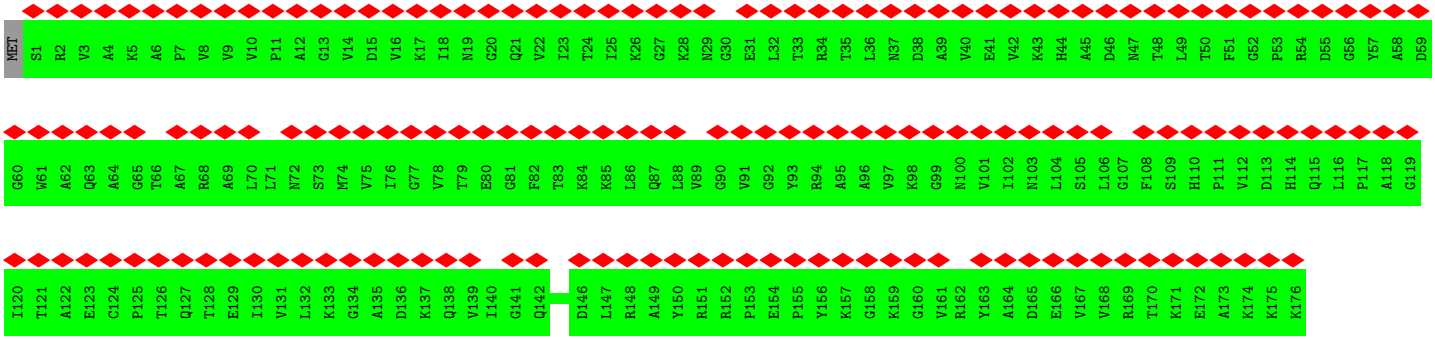




• Molecule 14: 50S ribosomal protein L6

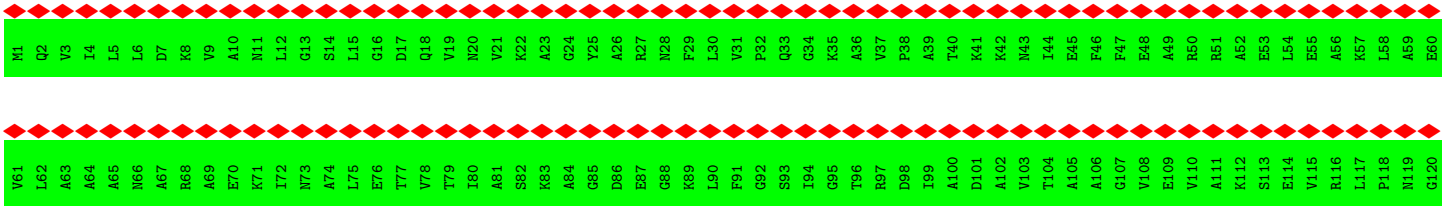
Chain G:

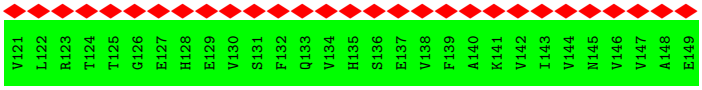




• Molecule 15: 50S ribosomal protein L9

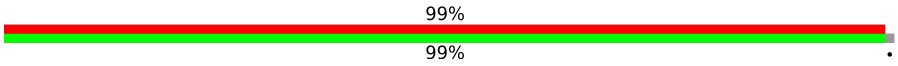
Chain H:

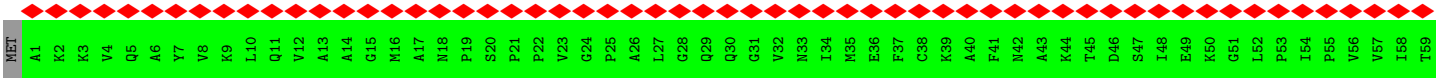


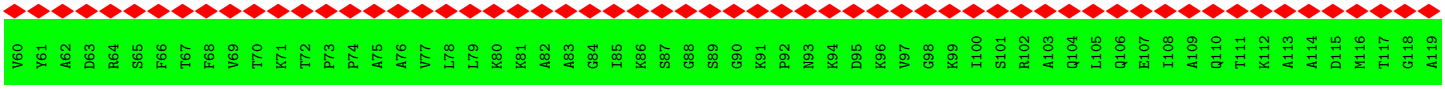


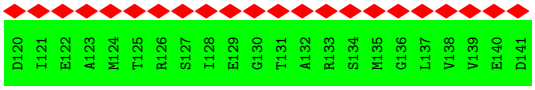
• Molecule 16: 50S ribosomal protein L11

Chain I:



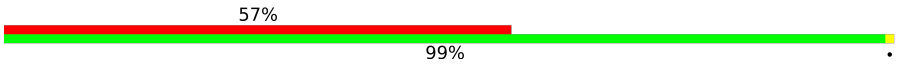


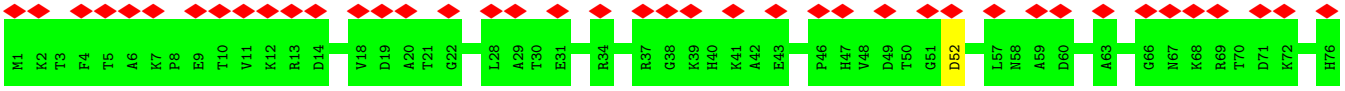




• Molecule 17: 50S ribosomal protein L13

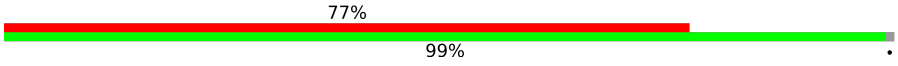
Chain J:

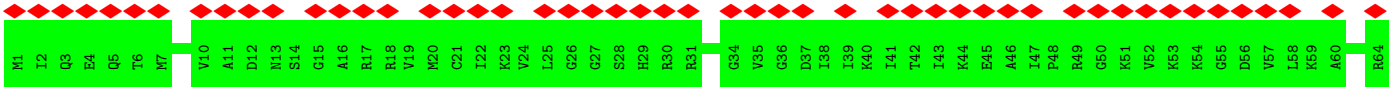




• Molecule 18: 50S ribosomal protein L14

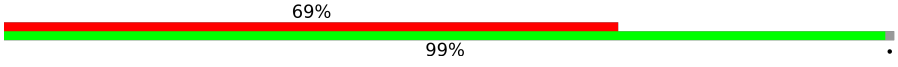
Chain K:

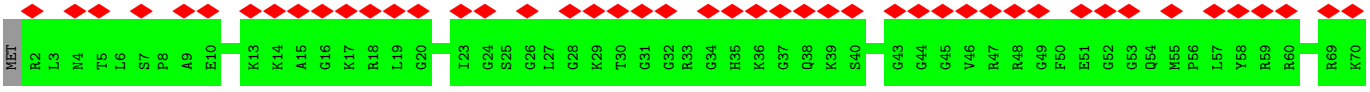


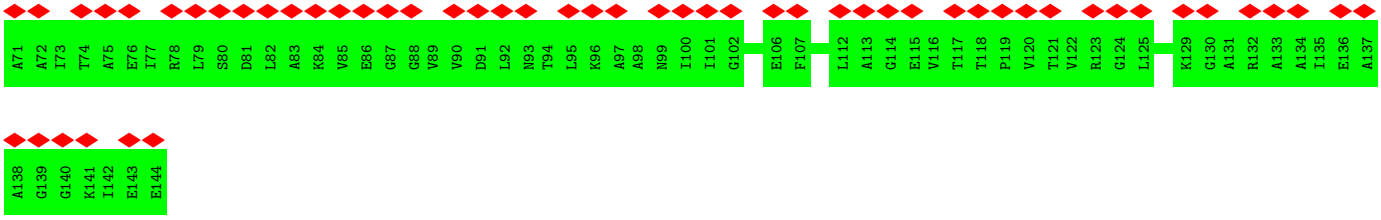


• Molecule 19: 50S ribosomal protein L15

Chain L:

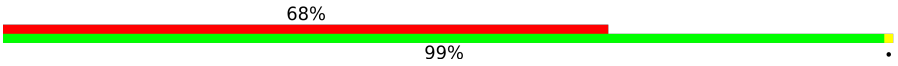


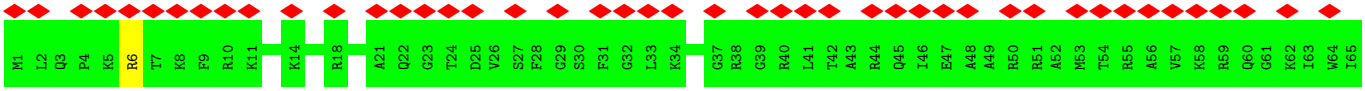




• Molecule 20: 50S ribosomal protein L16

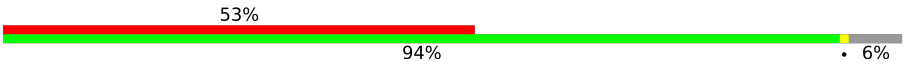
Chain M:

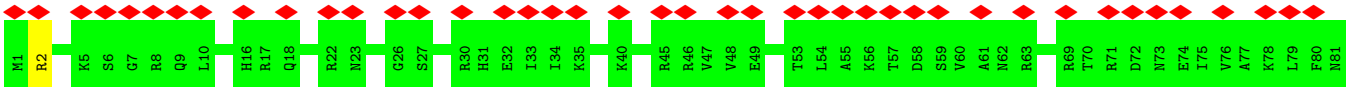


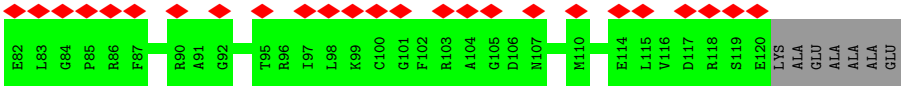


• Molecule 21: 50S ribosomal protein L17

Chain N:

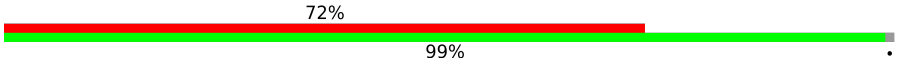


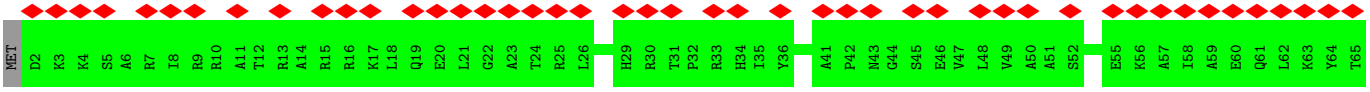




• Molecule 22: 50S ribosomal protein L18

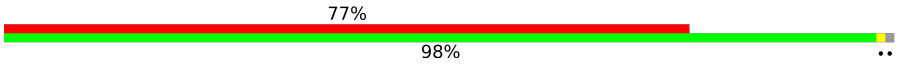
Chain O:

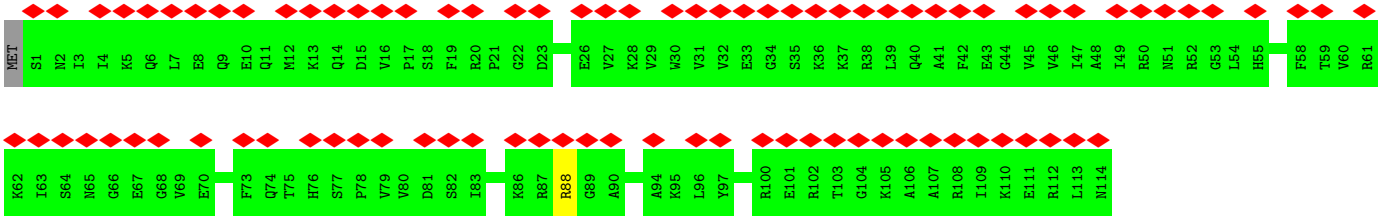




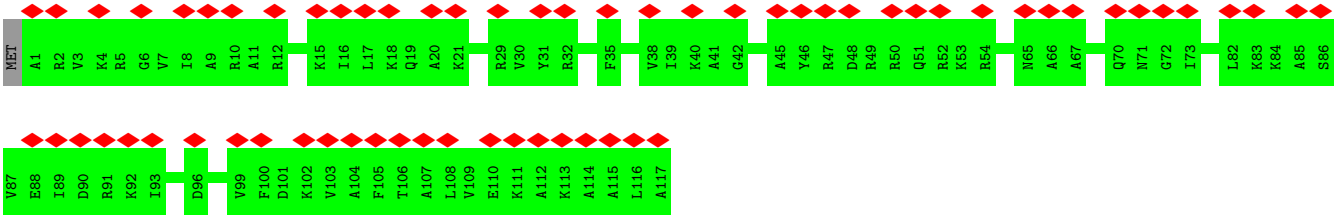
• Molecule 23: 50S ribosomal protein L19

Chain P:

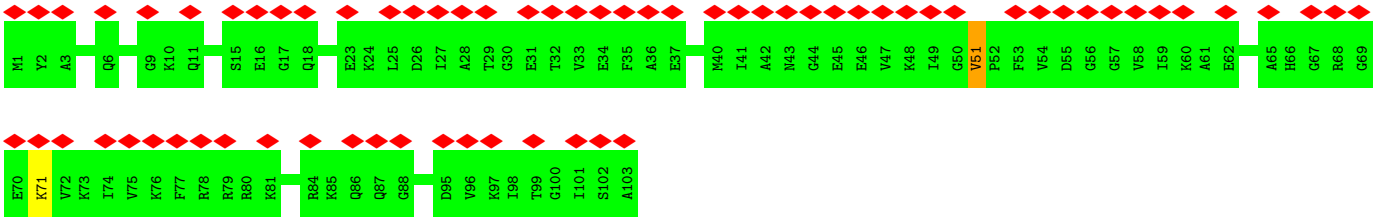




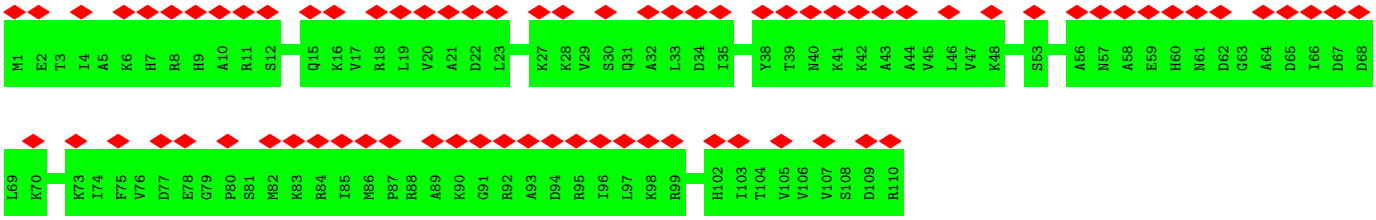
• Molecule 24: 50S ribosomal protein L20



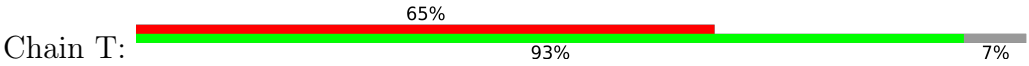
• Molecule 25: 50S ribosomal protein L21

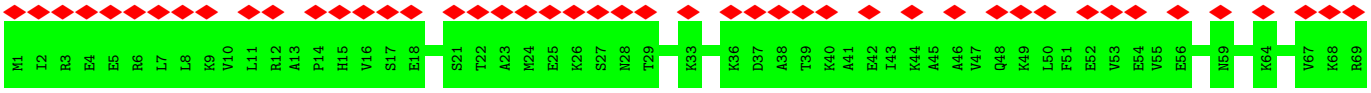


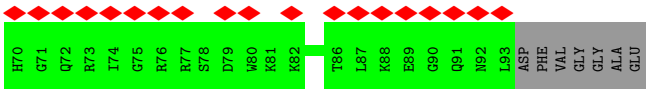
• Molecule 26: 50S ribosomal protein L22



• Molecule 27: 50S ribosomal protein L23

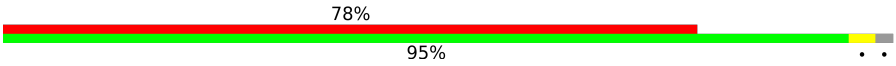


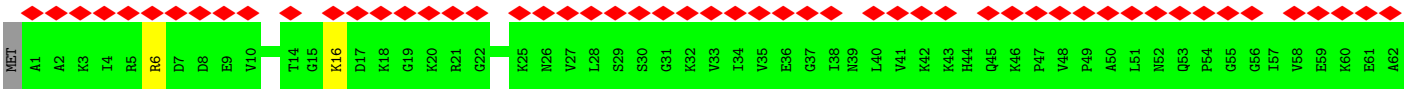


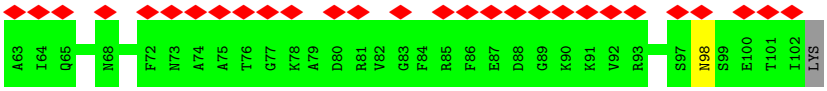


• Molecule 28: 50S ribosomal protein L24

Chain U:

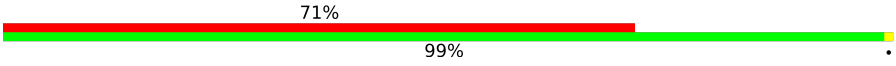


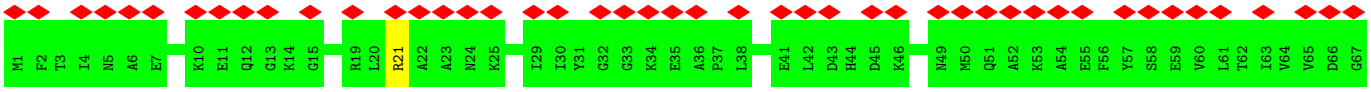


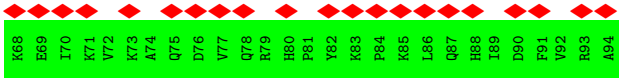


• Molecule 29: 50S ribosomal protein L25

Chain V:

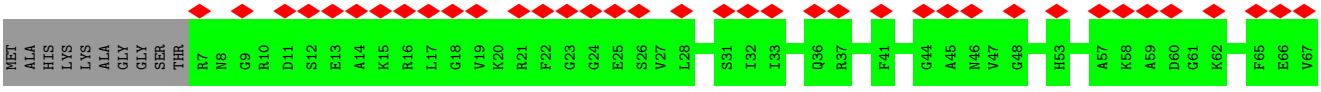


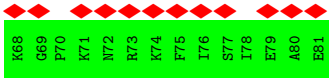




• Molecule 30: 50S ribosomal protein L27

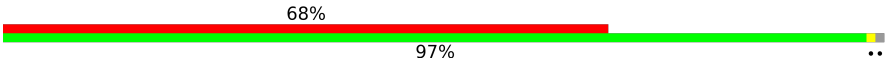
Chain W:

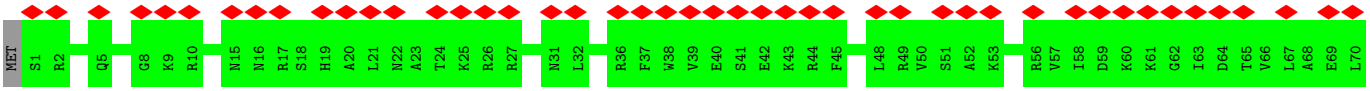


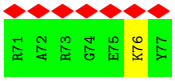


• Molecule 31: 50S ribosomal protein L28

Chain X:

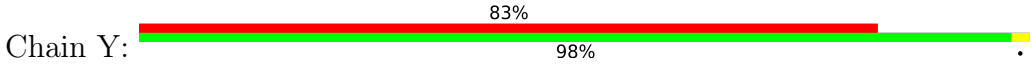


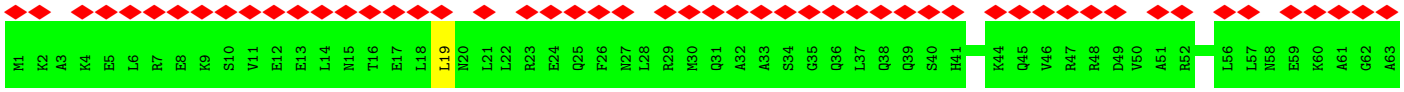




• Molecule 32: 50S ribosomal protein L29

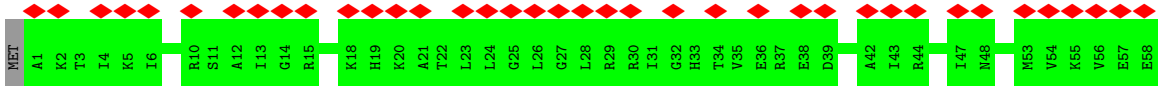
Chain Y:





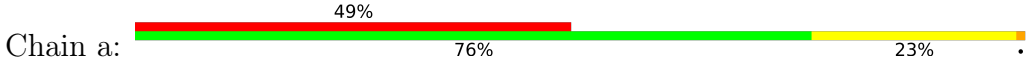
• Molecule 33: 50S ribosomal protein L30

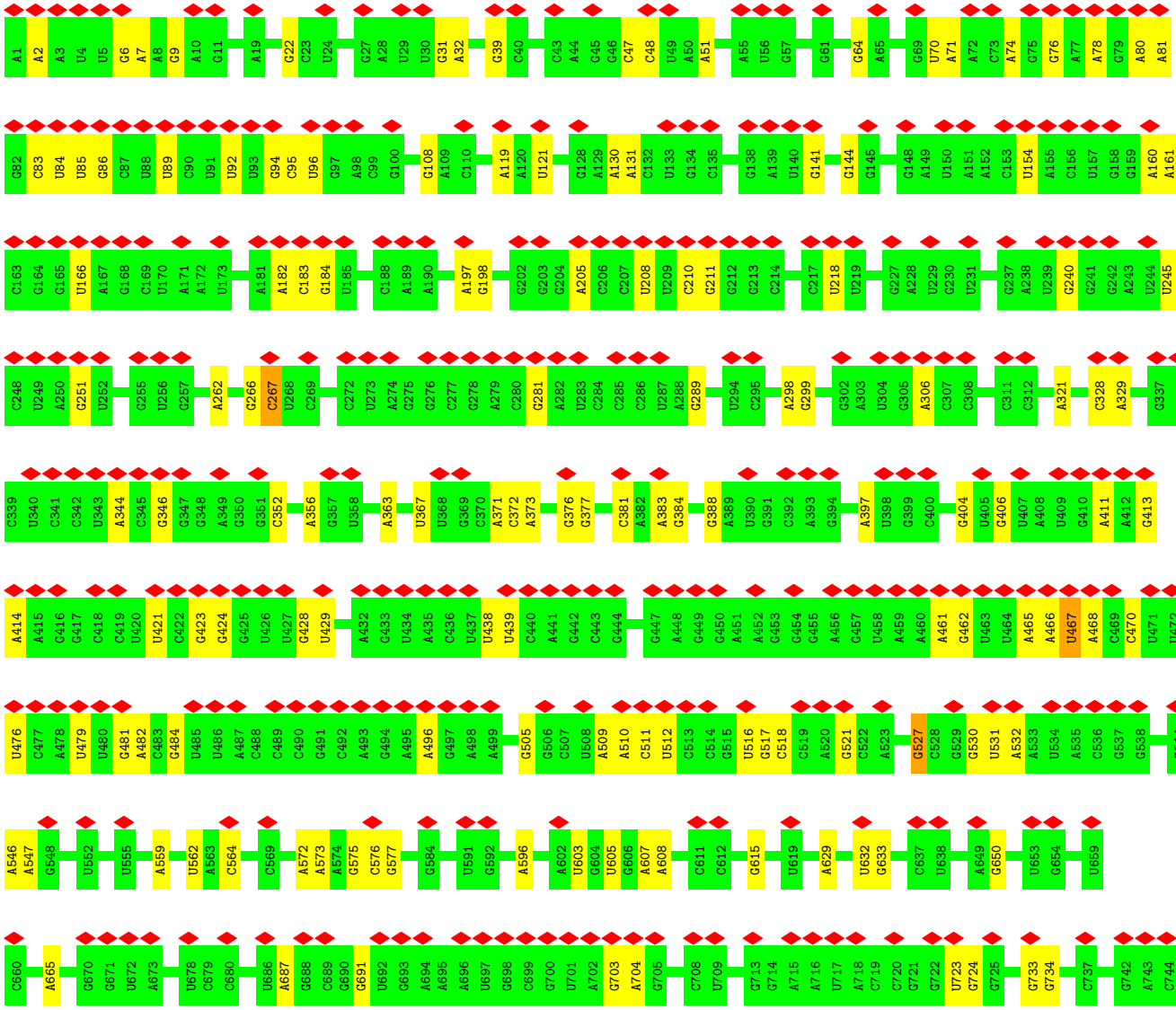
Chain Z:

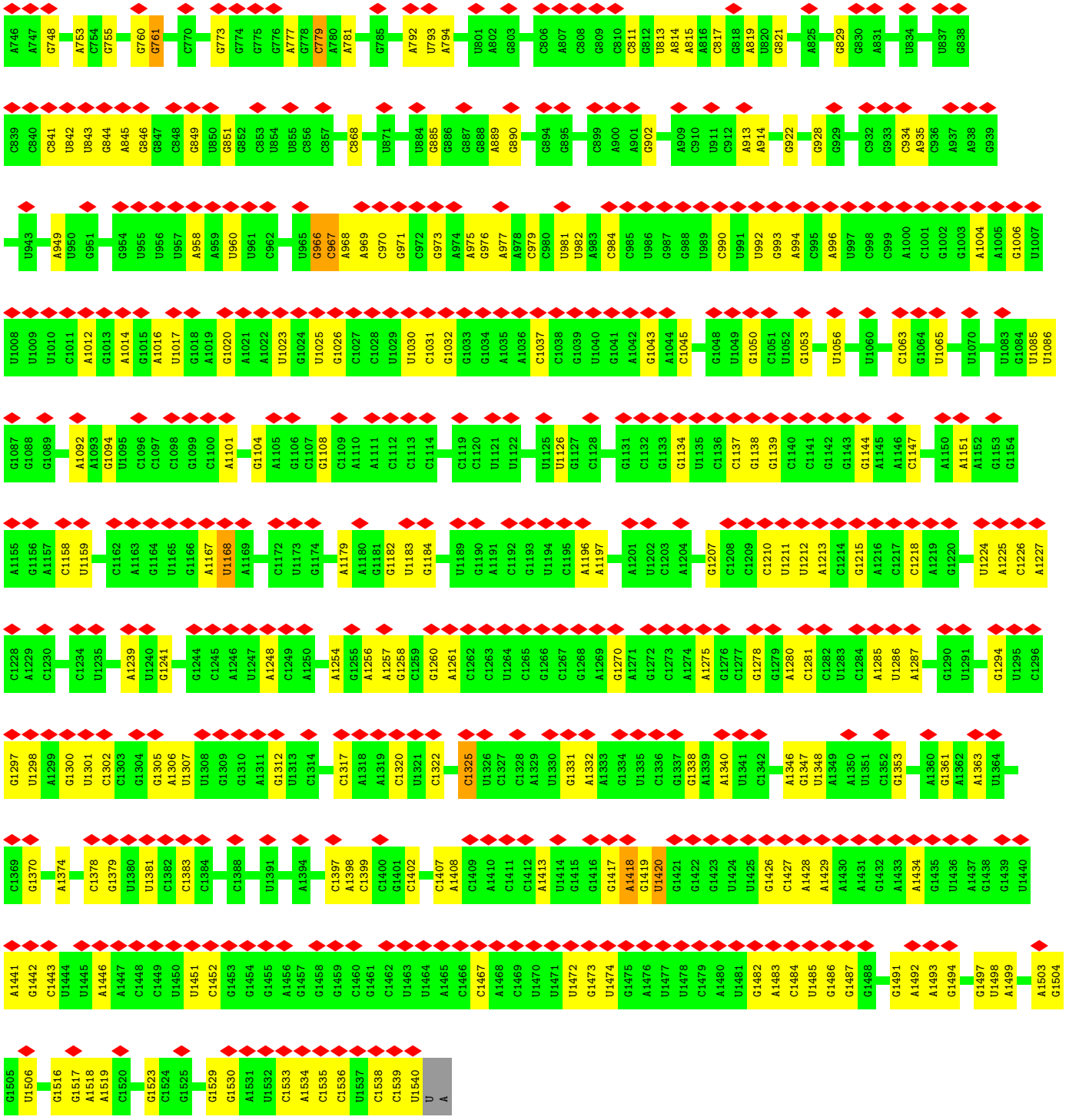


• Molecule 34: 16S ribosomal RNA

Chain a:

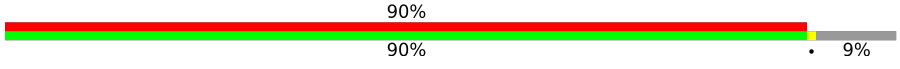


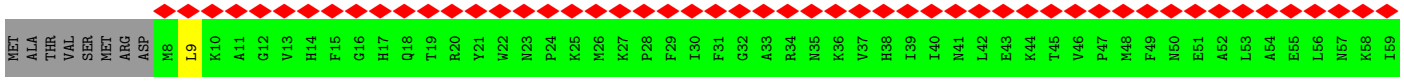


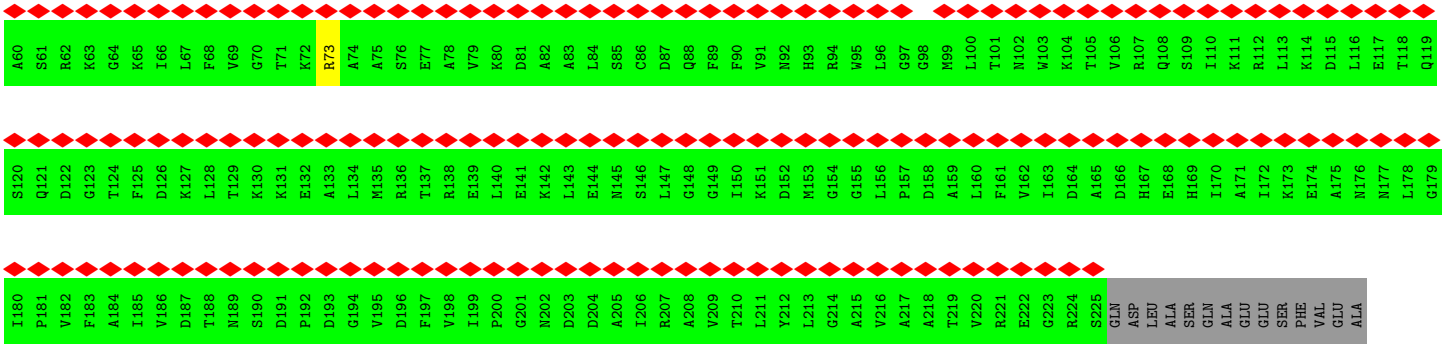


• Molecule 35: 30S ribosomal protein S2

Chain b:

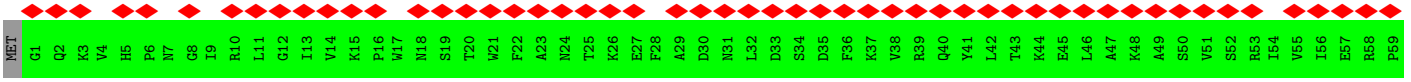


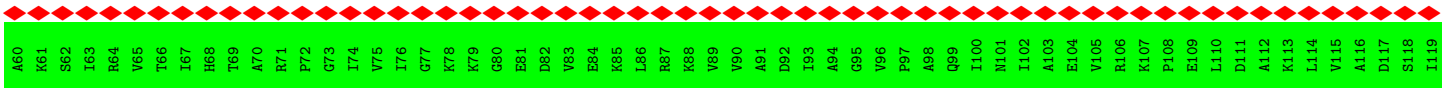




• Molecule 36: 30S ribosomal protein S3

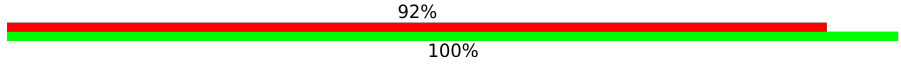
Chain c:

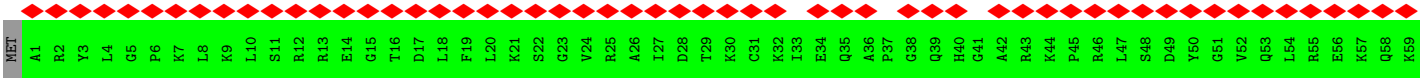




• Molecule 37: 30S ribosomal protein S4

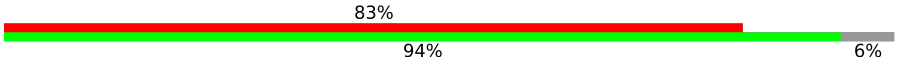
Chain d:

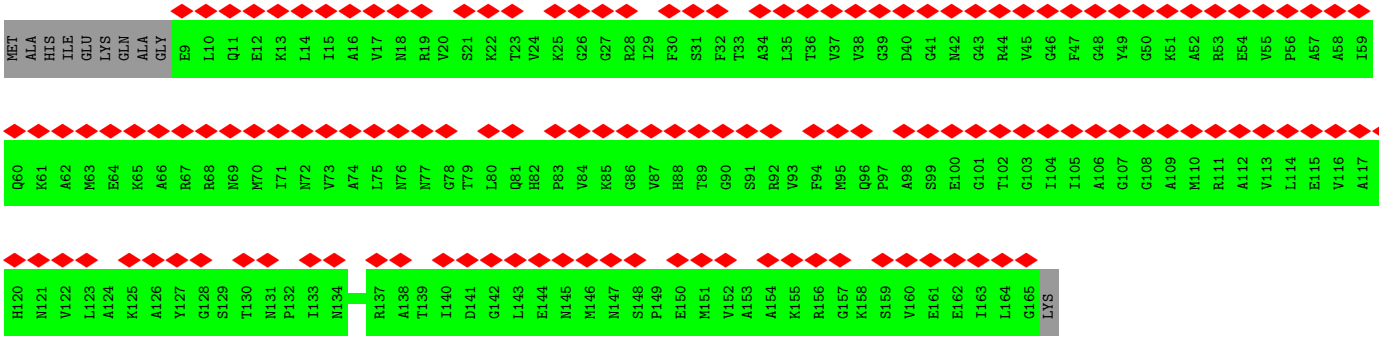




• Molecule 38: 30S ribosomal protein S5

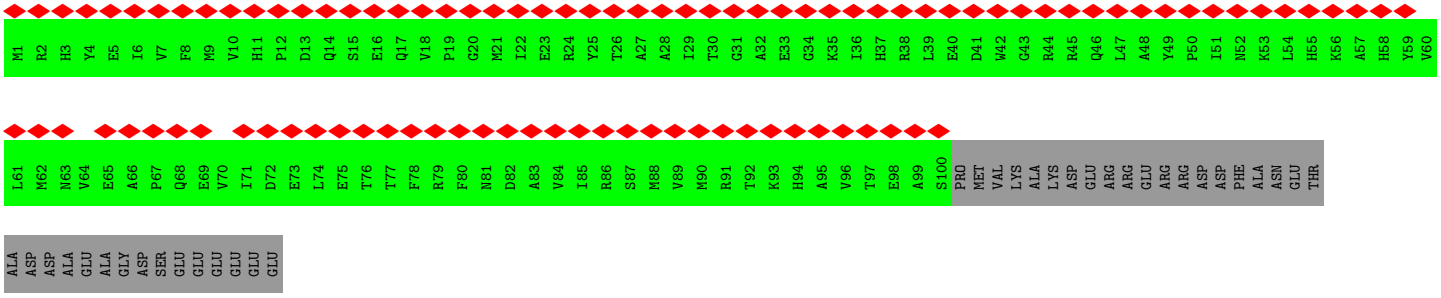
Chain e:





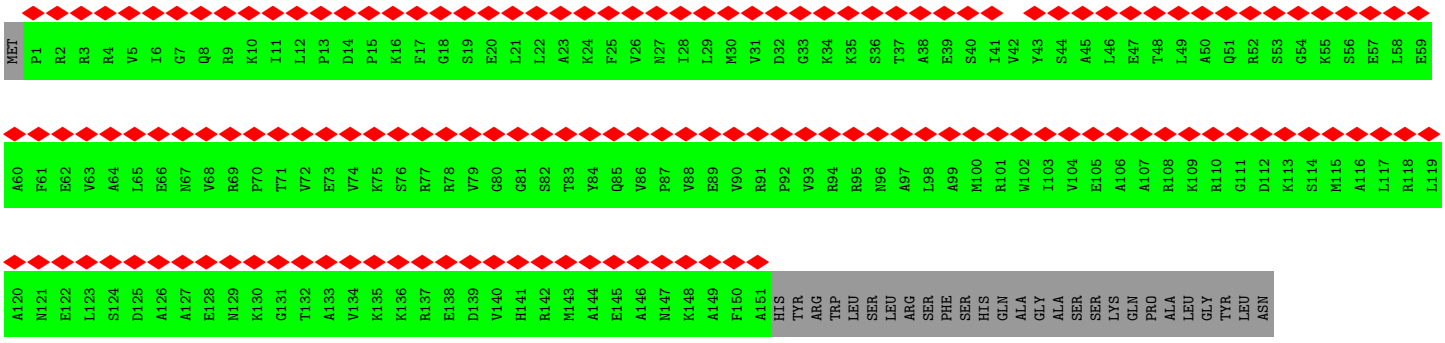
• Molecule 39: 30S ribosomal protein S6

Chain f:



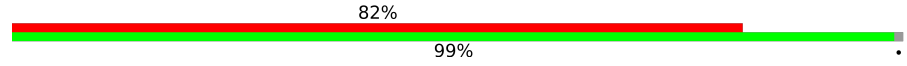
• Molecule 40: 30S ribosomal protein S7

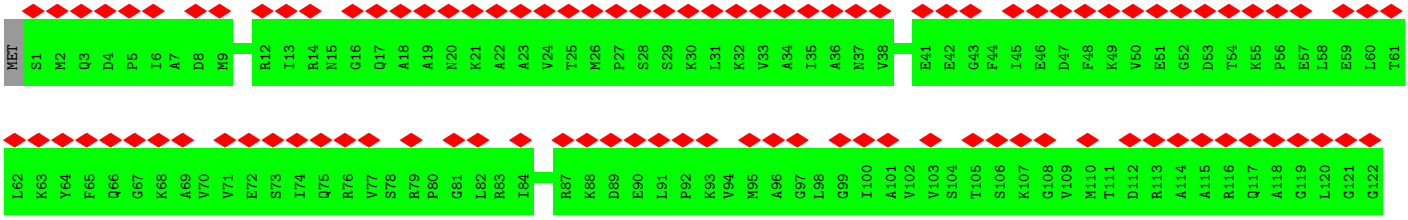
Chain g:

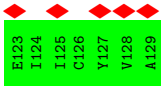


• Molecule 41: 30S ribosomal protein S8

Chain h:

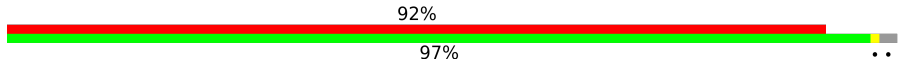


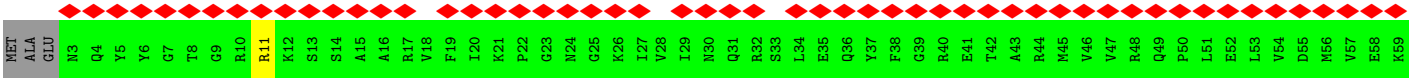


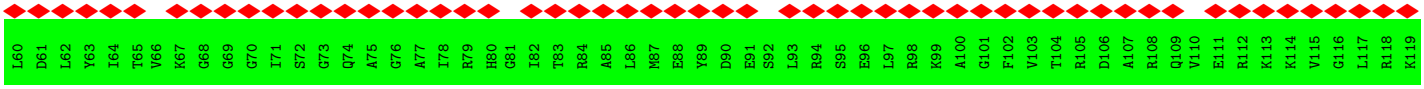


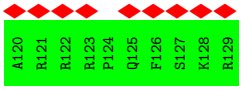
• Molecule 42: 30S ribosomal protein S9

Chain i:



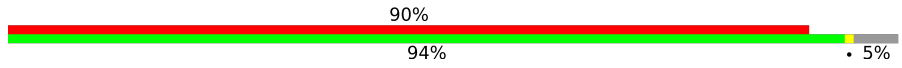


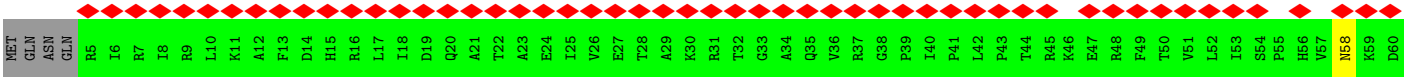


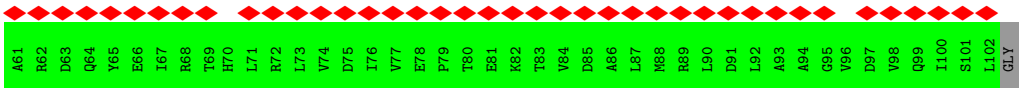


• Molecule 43: 30S ribosomal protein S10

Chain j:

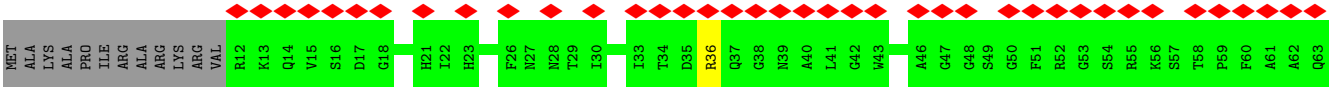


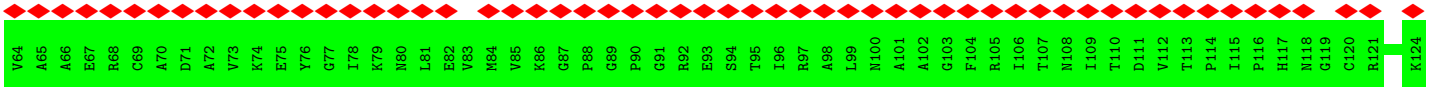




• Molecule 44: 30S ribosomal protein S11

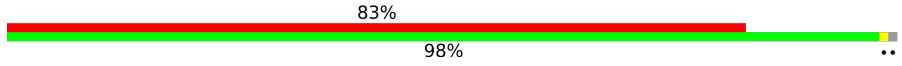
Chain k:





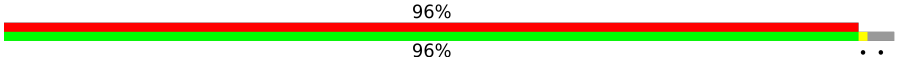
• Molecule 45: 30S ribosomal protein S12

Chain l:



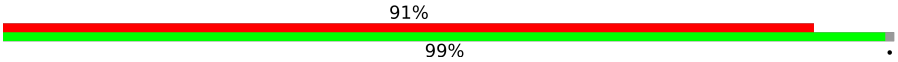
• Molecule 46: 30S ribosomal protein S13

Chain m:



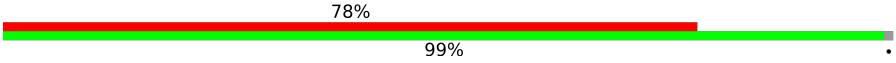
• Molecule 47: 30S ribosomal protein S14

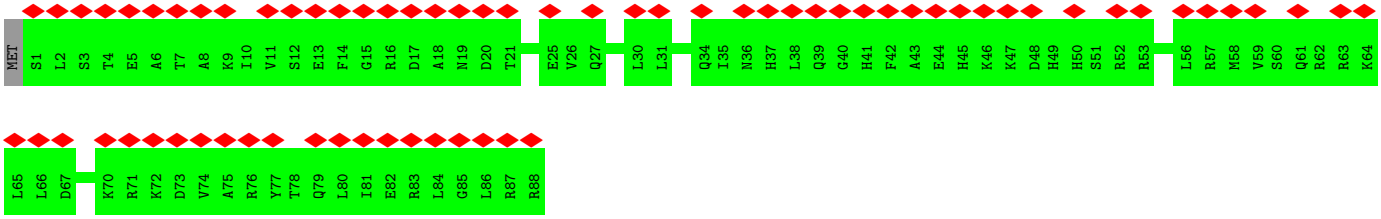
Chain n:



• Molecule 48: 30S ribosomal protein S15

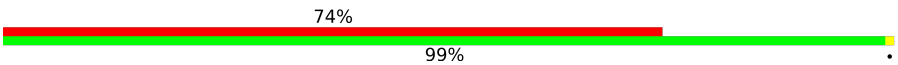
Chain o:

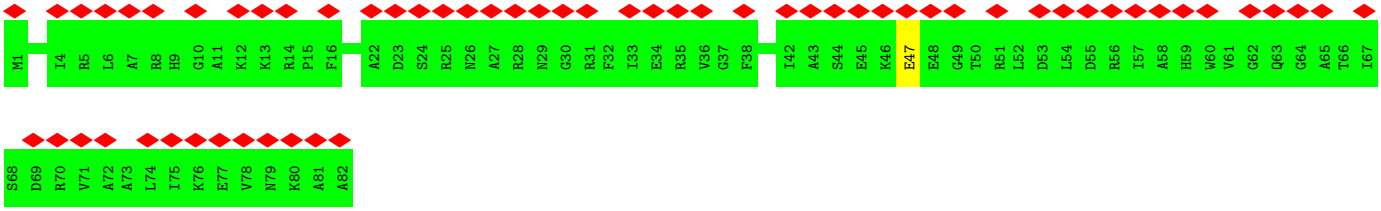




• Molecule 49: 30S ribosomal protein S16

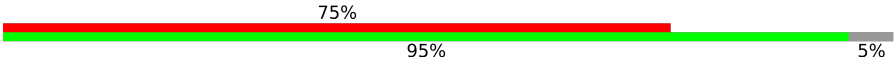
Chain p:

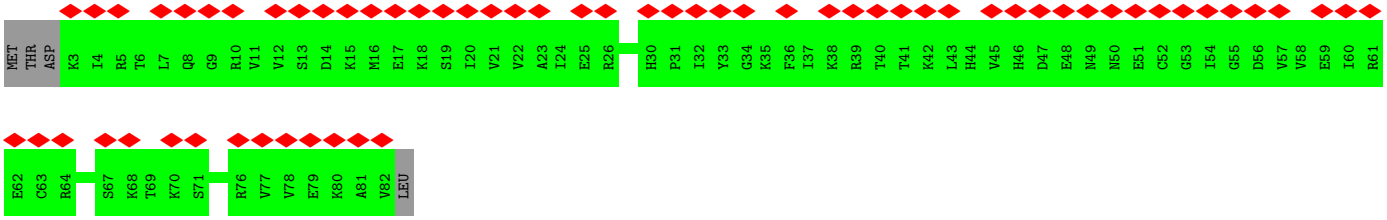




• Molecule 50: 30S ribosomal protein S17

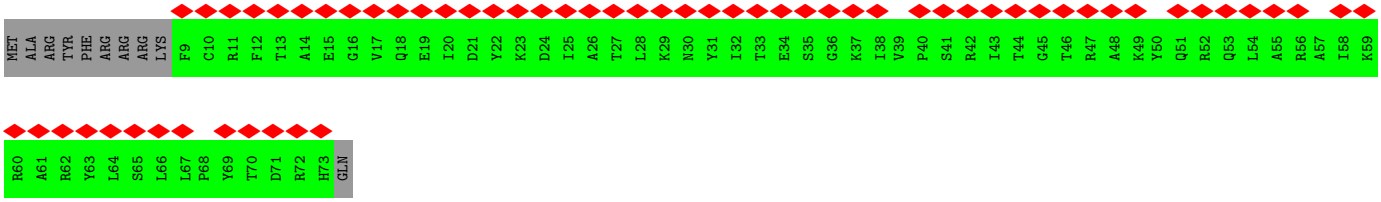
Chain q:





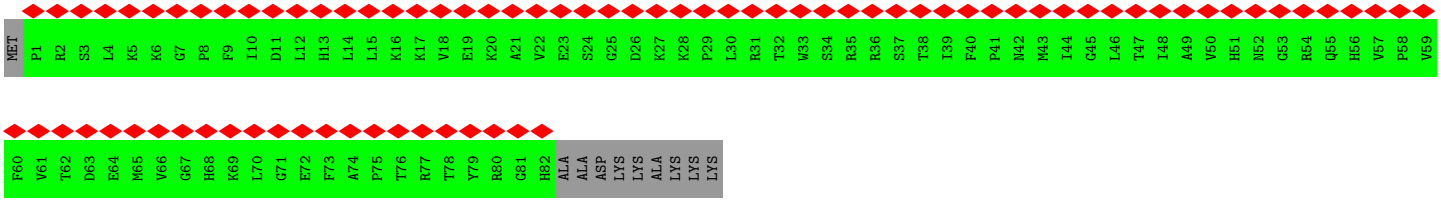
• Molecule 51: 30S ribosomal protein S18

Chain r:



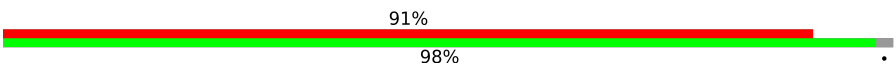
• Molecule 52: 30S ribosomal protein S19

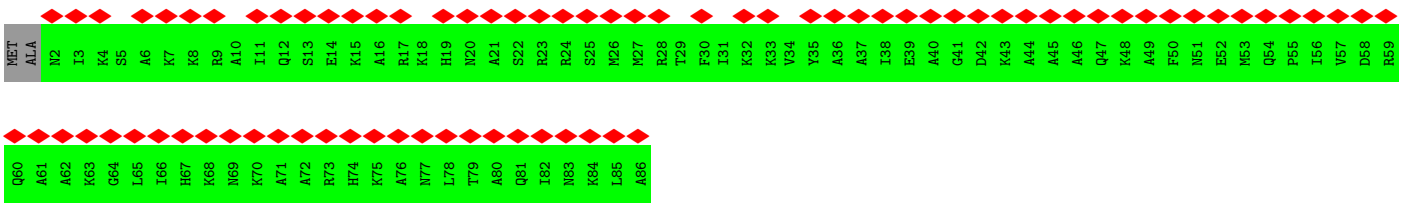
Chain s:



• Molecule 53: 30S ribosomal protein S20

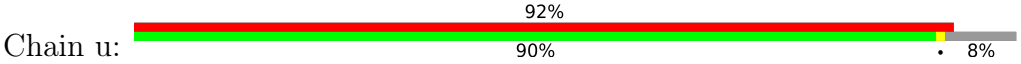
Chain t:





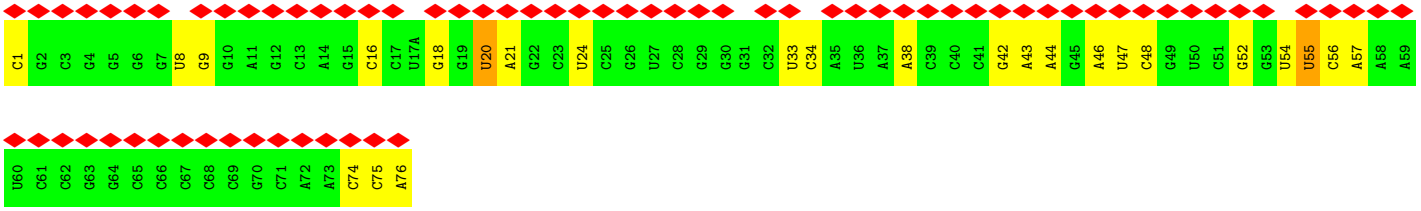
• Molecule 54: 30S ribosomal protein S21

Chain u:



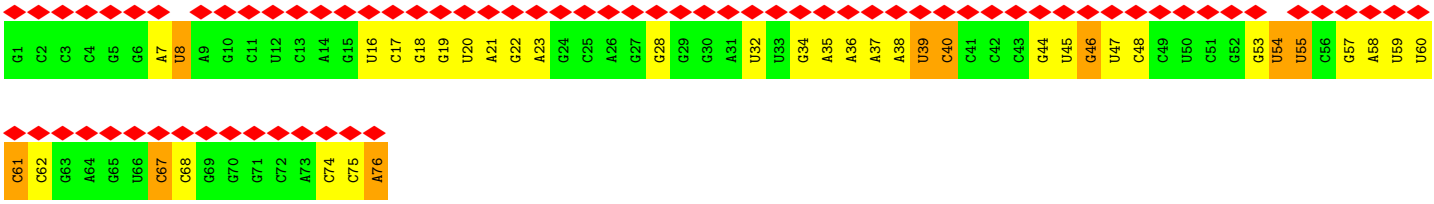
• Molecule 55: P-site tRNA(fMet)

Chain v:



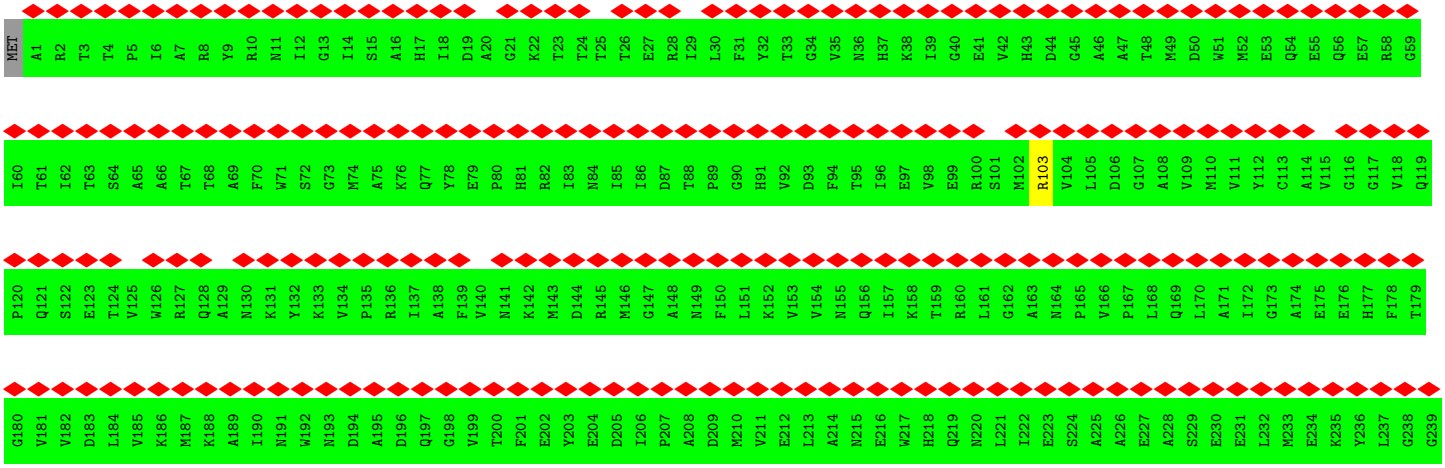
• Molecule 56: P-site fMet-Phe-tRNA(Phe)

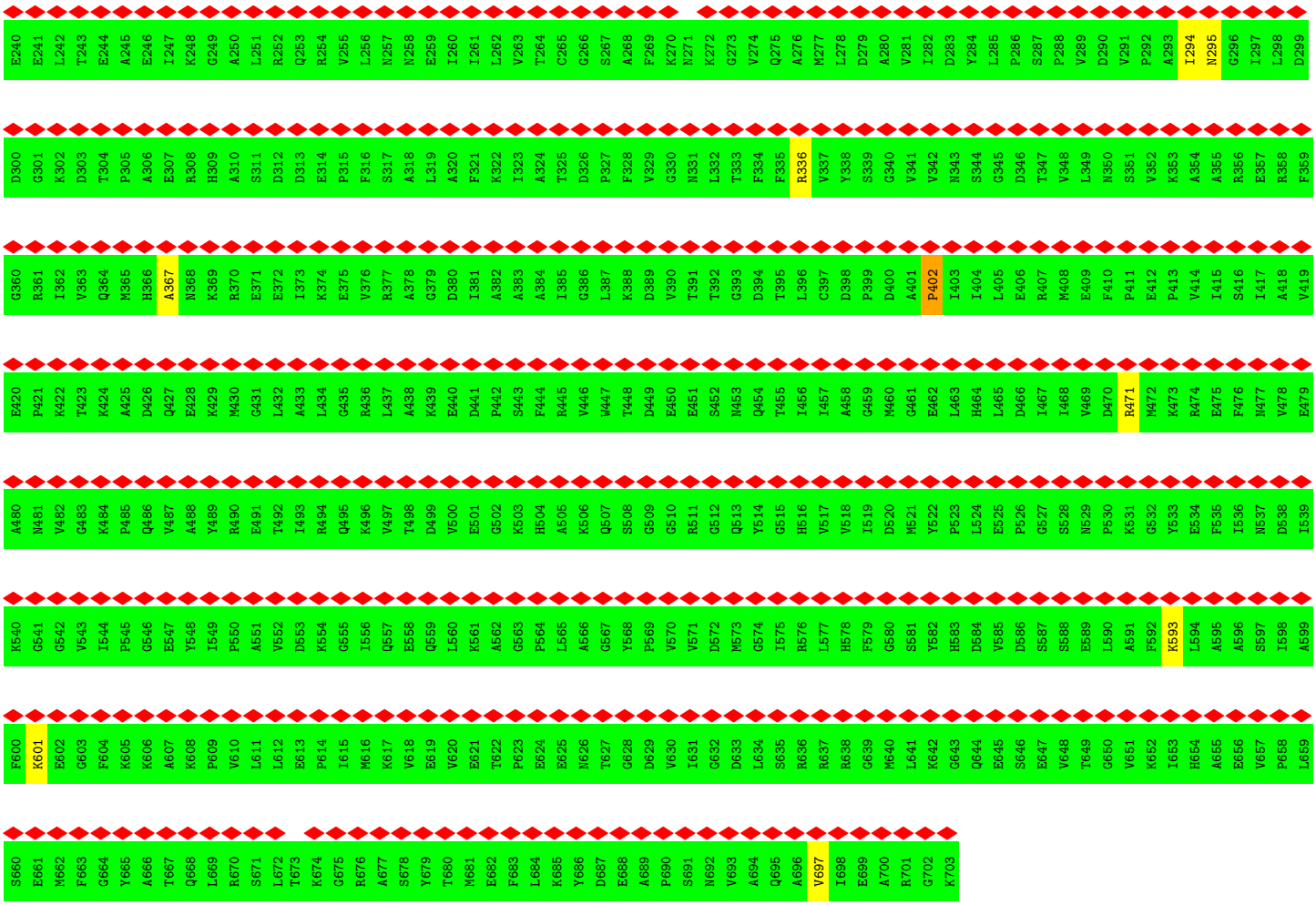
Chain w:



• Molecule 57: Elongation factor G

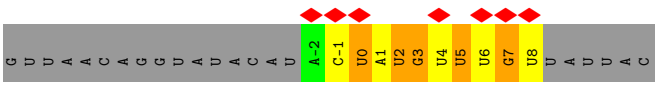
Chain x:





• Molecule 58: Dipeptide (FME-PHE)

• Molecule 59: mRNA



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	12.254	Depositor
Minimum map value	-7.636	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 3TD, MIA, 4SU, 5MC, UR3, 4OC, G7M, H2U, FME, 2MA, OMU, 1MG, PSU, OMC, 5MU, AM2, PO4, OMG, GDP, 2MG, 6MZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.39	0/450	0.52	0/599
2	1	0.38	0/416	0.46	0/554
3	2	0.41	0/380	0.53	0/498
4	3	0.47	0/513	0.62	0/676
5	4	0.39	0/303	0.53	0/397
6	5	0.25	0/646	0.50	0/898
7	6	0.45	0/531	0.58	0/709
8	A	0.82	2/69266 (0.0%)	1.00	75/108055 (0.1%)
9	B	0.71	1/2873 (0.0%)	0.90	0/4478
10	C	0.46	0/2121	0.54	0/2852
11	D	0.44	0/1586	0.53	0/2134
12	E	0.43	0/1571	0.53	0/2113
13	F	0.36	0/1434	0.51	0/1926
14	G	0.37	0/1343	0.49	0/1816
15	H	0.30	0/1122	0.57	0/1515
16	I	0.25	0/692	0.49	0/960
17	J	0.44	0/1152	0.49	0/1551
18	K	0.40	0/947	0.53	0/1268
19	L	0.41	0/1054	0.57	0/1403
20	M	0.41	0/1093	0.51	0/1460
21	N	0.43	0/973	0.55	0/1301
22	O	0.40	0/902	0.48	0/1209
23	P	0.44	0/929	0.53	0/1242
24	Q	0.55	0/960	0.52	0/1278
25	R	0.45	0/829	0.58	0/1107
26	S	0.41	0/864	0.56	0/1156
27	T	0.40	0/744	0.54	0/994
28	U	0.43	0/787	0.58	0/1051
29	V	0.42	0/766	0.48	0/1025
30	W	0.44	0/582	0.50	0/769
31	X	0.43	0/635	0.49	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Y	0.34	0/510	0.58	0/677
33	Z	0.38	0/453	0.53	0/605
34	a	0.69	1/36725 (0.0%)	0.97	30/57285 (0.1%)
35	b	0.32	0/1735	0.52	1/2338 (0.0%)
36	c	0.36	0/1651	0.50	0/2225
37	d	0.35	0/1665	0.51	0/2227
38	e	0.37	0/1154	0.52	0/1554
39	f	0.36	0/835	0.49	0/1128
40	g	0.30	0/1195	0.47	0/1602
41	h	0.41	0/989	0.56	0/1326
42	i	0.36	0/1034	0.54	0/1375
43	j	0.34	0/796	0.57	0/1077
44	k	0.37	0/885	0.52	0/1195
45	l	0.40	0/969	0.56	1/1300 (0.1%)
46	m	0.29	0/892	0.49	0/1193
47	n	0.30	0/811	0.44	0/1081
48	o	0.36	0/722	0.49	0/964
49	p	0.38	0/659	0.52	0/884
50	q	0.37	0/657	0.53	0/881
51	r	0.34	0/544	0.50	0/731
52	s	0.33	0/675	0.53	0/908
53	t	0.32	0/671	0.45	0/888
54	u	0.34	0/512	0.54	0/683
55	v	0.65	1/1745 (0.1%)	0.99	5/2716 (0.2%)
56	w	0.61	2/1650 (0.1%)	1.02	6/2569 (0.2%)
57	x	0.37	0/5546	0.55	1/7504 (0.0%)
58	y	0.46	0/11	2.19	0/13
59	z	1.26	2/255 (0.8%)	1.72	7/394 (1.8%)
All	All	0.67	9/164410 (0.0%)	0.88	126/245165 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	1	C	OP3-P	-10.88	1.48	1.61
9	B	1	U	OP3-P	-10.79	1.48	1.61
59	z	1	A	O3'-P	-10.73	1.48	1.61
8	A	1	G	OP3-P	-10.72	1.48	1.61
56	w	34	G	O3'-P	-9.32	1.50	1.61

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2103	C	N1-C2-O2	10.08	124.95	118.90
59	z	0	U	O5'-P-OP1	9.74	122.39	110.70
56	w	40	C	C2'-C3'-O3'	8.95	129.18	109.50
8	A	2103	C	N3-C2-O2	-8.93	115.65	121.90
8	A	2103	C	C2-N1-C1'	8.18	127.79	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
2	1	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
4	3	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
5	4	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
6	5	129/165 (78%)	98 (76%)	31 (24%)	0	100	100
7	6	64/70 (91%)	53 (83%)	11 (17%)	0	100	100
10	C	269/273 (98%)	229 (85%)	39 (14%)	1 (0%)	34	71
11	D	207/209 (99%)	172 (83%)	35 (17%)	0	100	100
12	E	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
13	F	175/179 (98%)	143 (82%)	32 (18%)	0	100	100
14	G	174/177 (98%)	154 (88%)	20 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	H	147/149 (99%)	117 (80%)	30 (20%)	0	100	100
16	I	139/142 (98%)	103 (74%)	36 (26%)	0	100	100
17	J	140/142 (99%)	128 (91%)	12 (9%)	0	100	100
18	K	120/123 (98%)	98 (82%)	22 (18%)	0	100	100
19	L	141/144 (98%)	113 (80%)	28 (20%)	0	100	100
20	M	134/136 (98%)	114 (85%)	20 (15%)	0	100	100
21	N	118/127 (93%)	106 (90%)	12 (10%)	0	100	100
22	O	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
23	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
24	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
25	R	101/103 (98%)	86 (85%)	13 (13%)	2 (2%)	7	40
26	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
27	T	91/100 (91%)	79 (87%)	12 (13%)	0	100	100
28	U	100/104 (96%)	85 (85%)	13 (13%)	2 (2%)	7	40
29	V	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
30	W	73/85 (86%)	60 (82%)	13 (18%)	0	100	100
31	X	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
32	Y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	44
33	Z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
35	b	216/240 (90%)	186 (86%)	30 (14%)	0	100	100
36	c	204/233 (88%)	185 (91%)	19 (9%)	0	100	100
37	d	203/206 (98%)	167 (82%)	36 (18%)	0	100	100
38	e	155/167 (93%)	134 (86%)	21 (14%)	0	100	100
39	f	98/135 (73%)	84 (86%)	14 (14%)	0	100	100
40	g	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
41	h	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
42	i	125/130 (96%)	104 (83%)	21 (17%)	0	100	100
43	j	96/103 (93%)	75 (78%)	20 (21%)	1 (1%)	15	53
44	k	114/129 (88%)	97 (85%)	17 (15%)	0	100	100
45	l	121/124 (98%)	95 (78%)	26 (22%)	0	100	100
46	m	112/118 (95%)	96 (86%)	16 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	n	99/102 (97%)	83 (84%)	16 (16%)	0	100 100
48	o	86/89 (97%)	75 (87%)	11 (13%)	0	100 100
49	p	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	12 48
50	q	78/84 (93%)	68 (87%)	10 (13%)	0	100 100
51	r	63/75 (84%)	52 (82%)	11 (18%)	0	100 100
52	s	80/92 (87%)	64 (80%)	16 (20%)	0	100 100
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100 100
54	u	63/71 (89%)	51 (81%)	11 (18%)	1 (2%)	9 44
57	x	701/704 (100%)	625 (89%)	74 (11%)	2 (0%)	41 75
All	All	6551/6924 (95%)	5653 (86%)	887 (14%)	11 (0%)	50 79

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	U	98	ASN
28	U	16	LYS
57	x	402	PRO
25	R	71	LYS
32	Y	19	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	47/48 (98%)	47 (100%)	0	100 100
2	1	45/49 (92%)	45 (100%)	0	100 100
3	2	38/38 (100%)	38 (100%)	0	100 100
4	3	51/52 (98%)	51 (100%)	0	100 100
5	4	34/34 (100%)	34 (100%)	0	100 100
7	6	59/62 (95%)	48 (81%)	11 (19%)	1 10
10	C	216/218 (99%)	216 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	D	164/164 (100%)	164 (100%)	0	100	100
12	E	165/165 (100%)	165 (100%)	0	100	100
13	F	148/150 (99%)	148 (100%)	0	100	100
14	G	137/138 (99%)	137 (100%)	0	100	100
15	H	114/114 (100%)	114 (100%)	0	100	100
17	J	116/116 (100%)	115 (99%)	1 (1%)	78	88
18	K	103/104 (99%)	103 (100%)	0	100	100
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	108 (99%)	1 (1%)	78	88
21	N	100/103 (97%)	99 (99%)	1 (1%)	76	86
22	O	86/87 (99%)	86 (100%)	0	100	100
23	P	99/100 (99%)	98 (99%)	1 (1%)	76	86
24	Q	89/90 (99%)	89 (100%)	0	100	100
25	R	84/84 (100%)	83 (99%)	1 (1%)	71	84
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	80 (100%)	0	100	100
28	U	83/85 (98%)	82 (99%)	1 (1%)	71	84
29	V	78/78 (100%)	77 (99%)	1 (1%)	69	82
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	66 (98%)	1 (2%)	65	80
32	Y	55/55 (100%)	55 (100%)	0	100	100
33	Z	48/49 (98%)	48 (100%)	0	100	100
35	b	180/198 (91%)	179 (99%)	1 (1%)	86	92
36	c	170/190 (90%)	170 (100%)	0	100	100
37	d	172/173 (99%)	172 (100%)	0	100	100
38	e	114/126 (90%)	114 (100%)	0	100	100
39	f	87/116 (75%)	87 (100%)	0	100	100
40	g	124/147 (84%)	124 (100%)	0	100	100
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	105/107 (98%)	104 (99%)	1 (1%)	76	86
43	j	86/90 (96%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	k	89/99 (90%)	88 (99%)	1 (1%)	73 85
45	l	103/104 (99%)	103 (100%)	0	100 100
46	m	92/96 (96%)	91 (99%)	1 (1%)	73 85
47	n	79/84 (94%)	79 (100%)	0	100 100
48	o	76/77 (99%)	76 (100%)	0	100 100
49	p	65/65 (100%)	65 (100%)	0	100 100
50	q	74/78 (95%)	74 (100%)	0	100 100
51	r	56/65 (86%)	56 (100%)	0	100 100
52	s	72/79 (91%)	72 (100%)	0	100 100
53	t	65/66 (98%)	65 (100%)	0	100 100
54	u	46/61 (75%)	46 (100%)	0	100 100
57	x	577/578 (100%)	569 (99%)	8 (1%)	67 81
58	y	1/1 (100%)	1 (100%)	0	100 100
All	All	5204/5408 (96%)	5173 (99%)	31 (1%)	86 92

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	P	88	ARG
57	x	471	ARG
29	V	21	ARG
57	x	601	LYS
57	x	294	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
50	q	46	HIS
57	x	427	GLN
52	s	13	HIS
53	t	47	GLN
57	x	559	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	347 (22%)	0
55	v	76/77 (98%)	21 (27%)	0
56	w	74/76 (97%)	35 (47%)	0
59	z	10/33 (30%)	8 (80%)	0
8	A	2898/2903 (99%)	717 (24%)	56 (1%)
9	B	119/120 (99%)	23 (19%)	3 (2%)
All	All	4713/4751 (99%)	1151 (24%)	59 (1%)

5 of 1151 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	12	U
8	A	15	G
8	A	27	G
8	A	35	G

5 of 59 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1490	A
8	A	2808	G
8	A	1917	PSU
8	A	2796	U
8	A	2505	G

5.4 Non-standard residues in protein, DNA, RNA chains (i)

46 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	OMG	A	2251	8	18,26,27	1.24	2 (11%)	20,38,41	2.13	6 (30%)
34	UR3	a	1498	34	14,22,23	2.72	4 (28%)	15,32,35	0.79	0
58	FME	y	101	58	8,9,10	0.48	0	7,9,11	1.04	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	2MA	A	2503	8	17,25,26	3.60	5 (29%)	19,37,40	1.61	3 (15%)
8	PSU	A	2580	8	17,21,22	1.34	3 (17%)	20,30,33	3.26	8 (40%)
34	5MC	a	967	34	15,22,23	3.14	5 (33%)	19,32,35	1.23	2 (10%)
34	2MG	a	1207	34	19,26,27	4.74	7 (36%)	21,38,41	2.09	8 (38%)
56	G7M	w	46	56	20,26,27	3.46	8 (40%)	20,39,42	2.48	5 (25%)
8	OMC	A	2498	8	15,22,23	0.93	0	17,31,34	1.40	2 (11%)
34	PSU	a	516	34	17,21,22	1.51	3 (17%)	20,30,33	3.07	7 (35%)
34	MA6	a	1518	34	19,26,27	1.04	1 (5%)	18,38,41	2.55	2 (11%)
34	G7M	a	527	34	20,26,27	3.39	8 (40%)	20,39,42	2.29	5 (25%)
56	4SU	w	8	56	14,21,22	3.37	5 (35%)	15,30,33	1.21	2 (13%)
55	H2U	v	20	55	18,21,22	3.03	5 (27%)	21,30,33	2.04	5 (23%)
8	OMU	A	2552	8	14,22,23	3.35	5 (35%)	14,31,34	0.70	0
34	MA6	a	1519	34	19,26,27	1.03	1 (5%)	18,38,41	2.66	2 (11%)
56	5MU	w	54	56	15,22,23	1.17	1 (6%)	16,32,35	2.06	3 (18%)
8	PSU	A	2604	8	17,21,22	1.23	3 (17%)	20,30,33	3.02	7 (35%)
8	3TD	A	1915	8	21,23,23	6.71	9 (42%)	26,35,35	5.02	12 (46%)
55	4SU	v	8	55	14,21,22	3.23	5 (35%)	15,30,33	1.14	2 (13%)
8	2MG	A	1835	8	19,26,27	4.75	8 (42%)	21,38,41	2.26	8 (38%)
34	4OC	a	1402	34	16,23,24	3.18	6 (37%)	17,32,35	1.16	1 (5%)
8	PSU	A	1917	8	17,21,22	3.21	6 (35%)	20,30,33	4.30	12 (60%)
8	PSU	A	746	8	17,21,22	1.25	3 (17%)	20,30,33	3.25	6 (30%)
8	5MC	A	747	8	15,22,23	2.93	5 (33%)	19,32,35	1.31	3 (15%)
8	PSU	A	2504	8	17,21,22	1.22	3 (17%)	20,30,33	3.08	6 (30%)
8	PSU	A	955	8	17,21,22	1.12	2 (11%)	20,30,33	3.21	5 (25%)
8	6MZ	A	1618	8	18,25,26	2.17	4 (22%)	16,36,39	2.03	3 (18%)
8	PSU	A	1911	8	17,21,22	1.11	3 (17%)	20,30,33	3.13	6 (30%)
34	2MG	a	1516	34	19,26,27	4.75	8 (42%)	21,38,41	2.29	7 (33%)
55	5MU	v	54	55	15,22,23	2.82	3 (20%)	16,32,35	2.79	2 (12%)
8	2MG	A	2445	8	19,26,27	1.19	2 (10%)	21,38,41	2.26	7 (33%)
8	1MG	A	745	8	18,26,27	3.48	5 (27%)	19,39,42	1.94	2 (10%)
8	6MZ	A	2030	8	18,25,26	1.28	2 (11%)	16,36,39	2.30	6 (37%)
8	G7M	A	2069	8	20,26,27	3.34	8 (40%)	20,39,42	2.42	5 (25%)
55	PSU	v	55	55	17,21,22	1.09	2 (11%)	20,30,33	3.17	5 (25%)
34	2MG	a	966	34	19,26,27	4.76	7 (36%)	21,38,41	2.15	8 (38%)
34	5MC	a	1407	34	15,22,23	3.07	5 (33%)	19,32,35	1.41	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	PSU	w	55	56	17,21,22	1.55	3 (17%)	20,30,33	3.19	7 (35%)
8	PSU	A	2457	8	17,21,22	1.69	3 (17%)	20,30,33	3.11	6 (30%)
56	PSU	w	32	56	17,21,22	2.56	4 (23%)	20,30,33	4.14	11 (55%)
56	MIA	w	37	56	24,31,32	3.90	9 (37%)	26,44,47	3.57	14 (53%)
8	PSU	A	2605	8	17,21,22	1.17	3 (17%)	20,30,33	3.03	6 (30%)
56	PSU	w	39	56	17,21,22	3.05	5 (29%)	20,30,33	4.39	14 (70%)
8	5MC	A	1962	8	15,22,23	2.99	5 (33%)	19,32,35	1.60	4 (21%)
8	5MU	A	1939	8	15,22,23	2.85	3 (20%)	16,32,35	2.83	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OMG	A	2251	8	-	2/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	0/5/25/26	0/2/2/2
58	FME	y	101	58	-	4/7/9/11	-
8	2MA	A	2503	8	-	2/3/25/26	0/3/3/3
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	2/5/25/26	0/2/2/2
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
56	G7M	w	46	56	-	2/3/25/26	0/3/3/3
8	OMC	A	2498	8	-	1/7/27/28	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
34	G7M	a	527	34	-	2/3/25/26	0/3/3/3
56	4SU	w	8	56	-	0/5/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
8	OMU	A	2552	8	-	1/7/27/28	0/2/2/2
34	MA6	a	1519	34	-	3/7/29/30	0/3/3/3
56	5MU	w	54	56	-	1/5/25/26	0/2/2/2
8	PSU	A	2604	8	-	1/7/25/26	0/2/2/2
8	3TD	A	1915	8	-	4/10/26/26	0/2/2/2
55	4SU	v	8	55	-	1/5/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
34	4OC	a	1402	34	-	3/9/29/30	0/2/2/2
8	PSU	A	1917	8	-	5/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PSU	A	746	8	-	4/7/25/26	0/2/2/2
8	5MC	A	747	8	-	0/5/25/26	0/2/2/2
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	2/5/27/28	0/3/3/3
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
55	5MU	v	54	55	-	0/5/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
8	1MG	A	745	8	-	2/3/25/26	0/3/3/3
8	6MZ	A	2030	8	-	5/5/27/28	0/3/3/3
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
55	PSU	v	55	55	-	3/7/25/26	0/2/2/2
34	2MG	a	966	34	-	2/5/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/5/25/26	0/2/2/2
56	PSU	w	55	56	-	2/7/25/26	0/2/2/2
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	3/7/25/26	0/2/2/2
56	MIA	w	37	56	-	6/11/33/34	0/3/3/3
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	5/7/25/26	0/2/2/2
8	5MC	A	1962	8	-	2/5/25/26	0/2/2/2
8	5MU	A	1939	8	-	2/5/25/26	0/2/2/2

The worst 5 of 197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C2'-C1'	-21.88	1.28	1.54
34	a	1516	2MG	C2-N2	15.74	1.47	1.34
34	a	1207	2MG	C2-N2	15.51	1.47	1.34
8	A	1835	2MG	C2-N2	15.49	1.47	1.34
34	a	966	2MG	C2-N2	15.35	1.47	1.34

The worst 5 of 241 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1915	3TD	C5-C1'-C2'	-12.76	92.56	115.32
8	A	1915	3TD	O9-P-O5'	-12.58	73.25	106.73
8	A	746	PSU	N1-C2-N3	-11.07	119.63	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	955	PSU	N1-C2-N3	-11.00	119.69	128.43
55	v	55	PSU	N1-C2-N3	-10.72	119.91	128.43

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
8	A	745	1MG	O4'-C4'-C5'-O5'
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	O4'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	GDP	x	801	-	24,30,30	1.13	2 (8%)	31,47,47	2.27	10 (32%)
60	AM2	a	2001	-	40,40,40	0.83	1 (2%)	53,60,60	1.73	12 (22%)
61	PO4	x	802	-	4,4,4	1.11	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GDP	x	801	-	-	5/12/32/32	0/3/3/3
60	AM2	a	2001	-	-	4/12/84/84	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	x	801	GDP	C6-C5	3.85	1.48	1.41
60	a	2001	AM2	CA6-CA7	-2.62	1.48	1.53
62	x	801	GDP	C5-C4	2.02	1.46	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	x	801	GDP	PA-O3A-PB	-5.36	114.44	132.83
62	x	801	GDP	C2-N3-C4	5.01	121.07	115.36
62	x	801	GDP	C6-C5-C4	-4.61	116.40	120.80
60	a	2001	AM2	OA6-CA6-CA7	-4.20	101.18	109.66
60	a	2001	AM2	CA8-CA7-CA6	-3.87	98.68	110.06

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	x	801	GDP	C5'-O5'-PA-O1A
62	x	801	GDP	C5'-O5'-PA-O2A
60	a	2001	AM2	OB1-CB5-CB6-OB6
62	x	801	GDP	O4'-C4'-C5'-O5'
60	a	2001	AM2	CB4-CB5-CB6-OB6

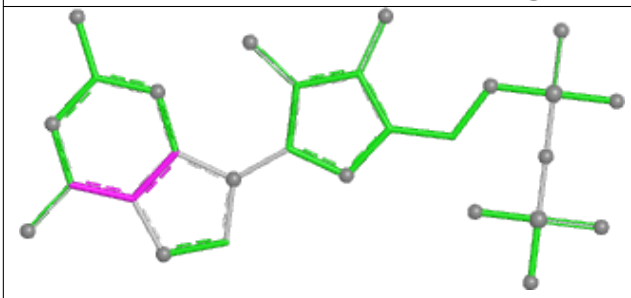
There are no ring outliers.

No monomer is involved in short contacts.

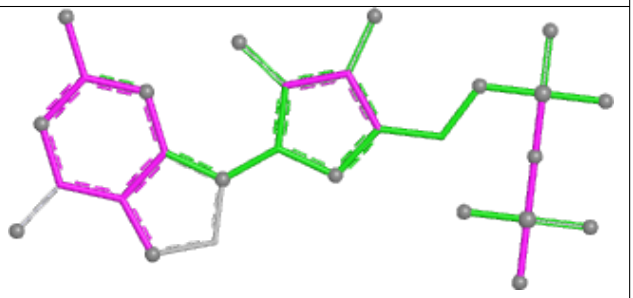
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

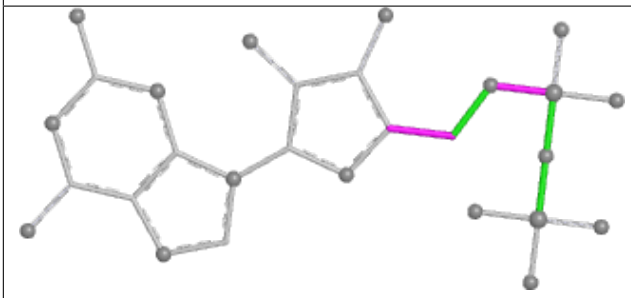
Ligand GDP x 801



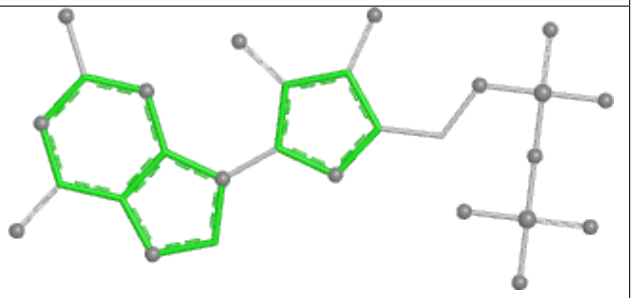
Bond lengths



Bond angles

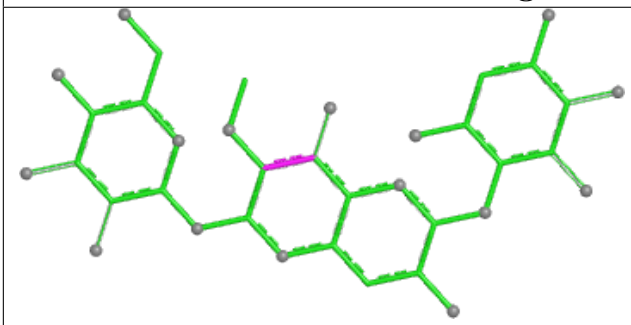


Torsions

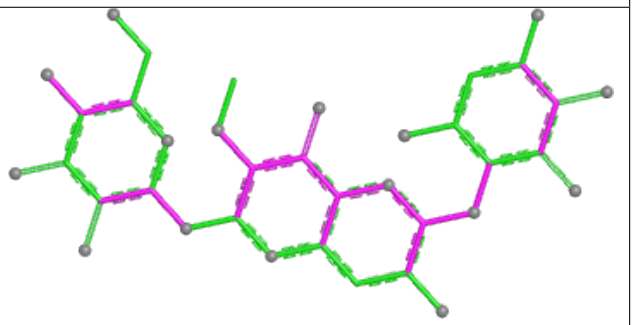


Rings

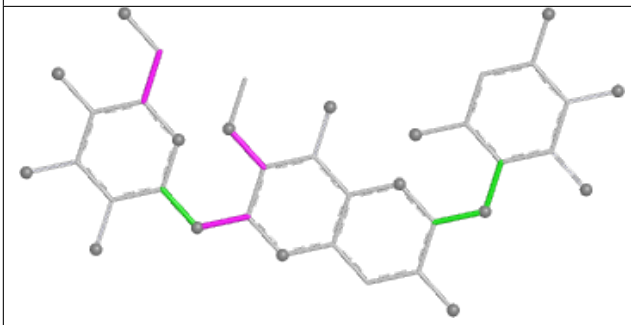
Ligand AM2 a 2001



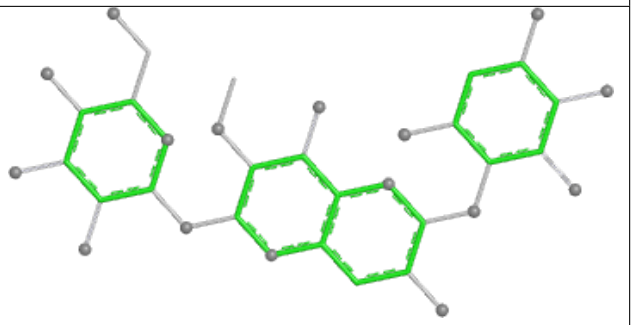
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

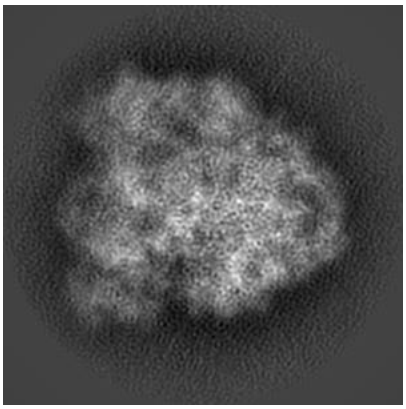
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13462. These allow visual inspection of the internal detail of the map and identification of artifacts.

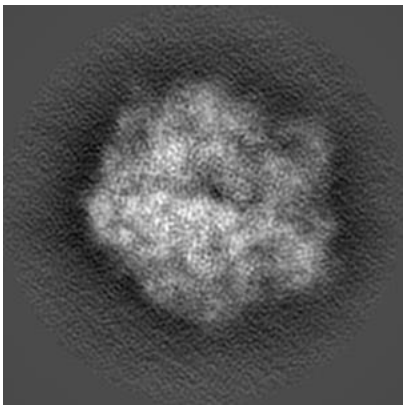
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

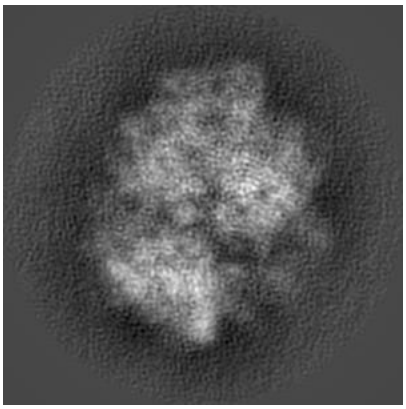
6.1.1 Primary map



X

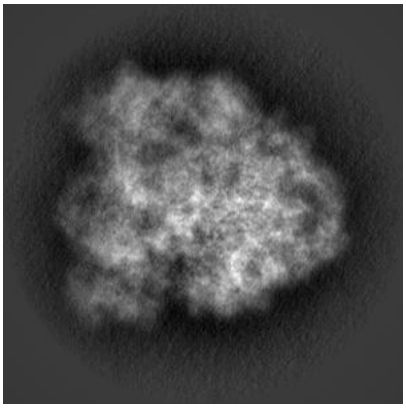


Y

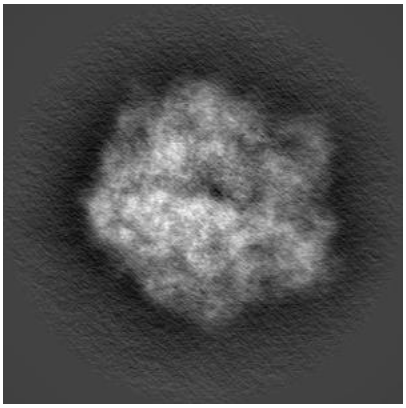


Z

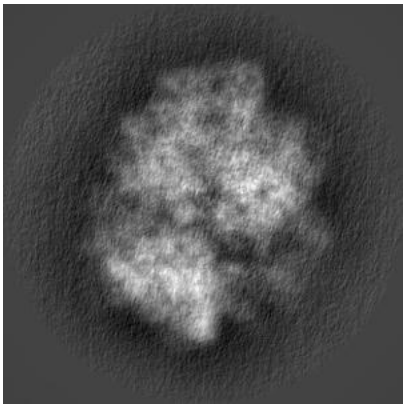
6.1.2 Raw map



X



Y

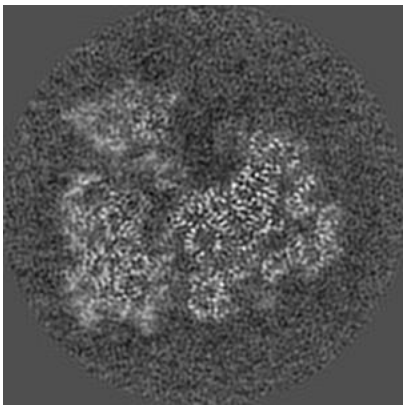


Z

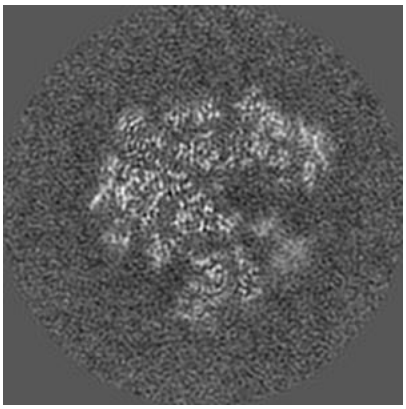
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

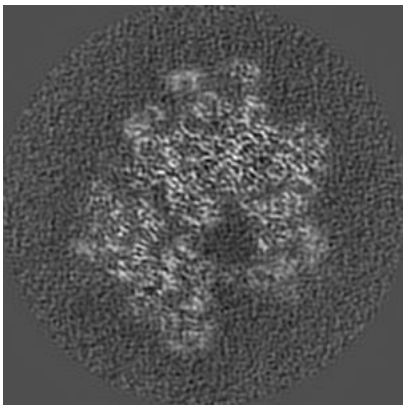
6.2.1 Primary map



X Index: 144

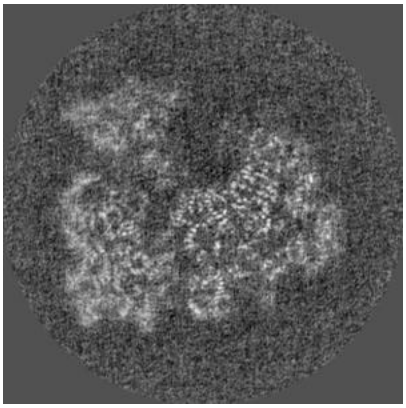


Y Index: 144

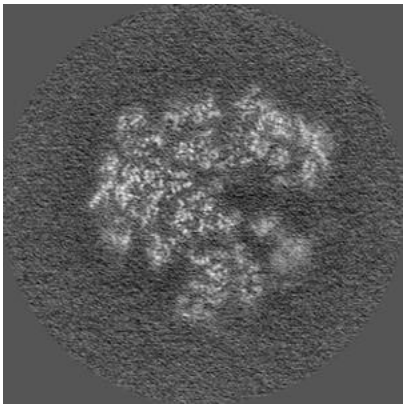


Z Index: 144

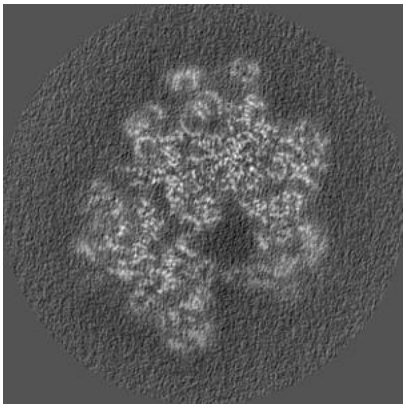
6.2.2 Raw map



X Index: 144



Y Index: 144

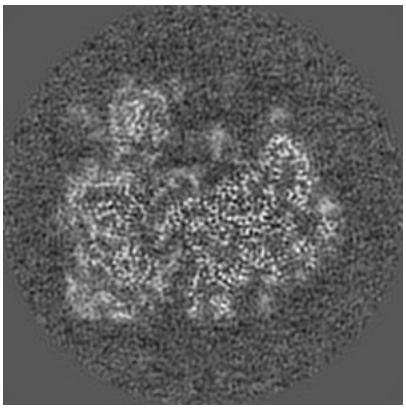


Z Index: 144

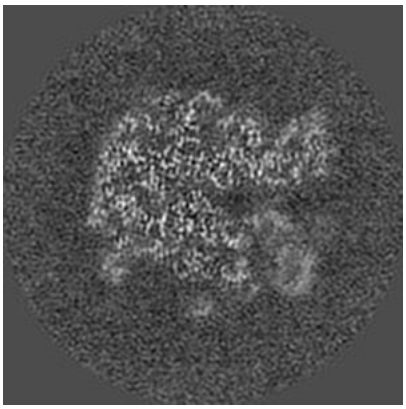
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

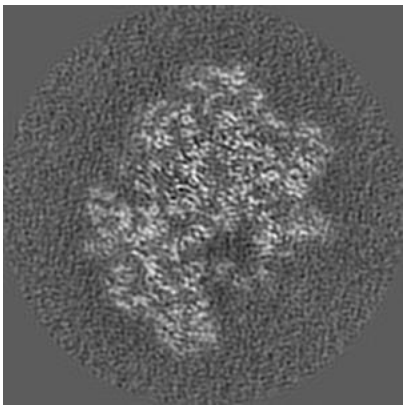
6.3.1 Primary map



X Index: 138

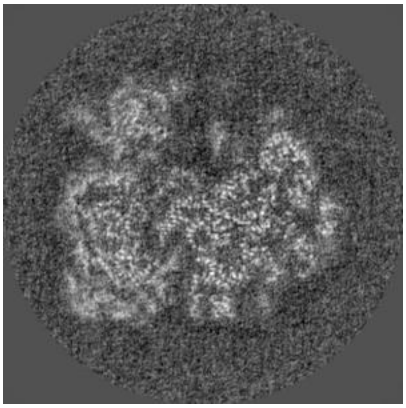


Y Index: 157

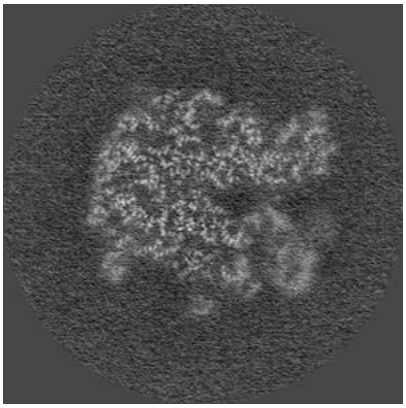


Z Index: 134

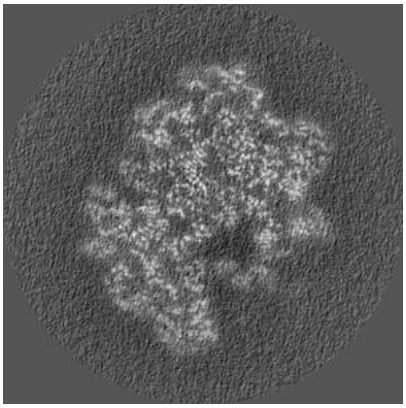
6.3.2 Raw map



X Index: 139



Y Index: 157

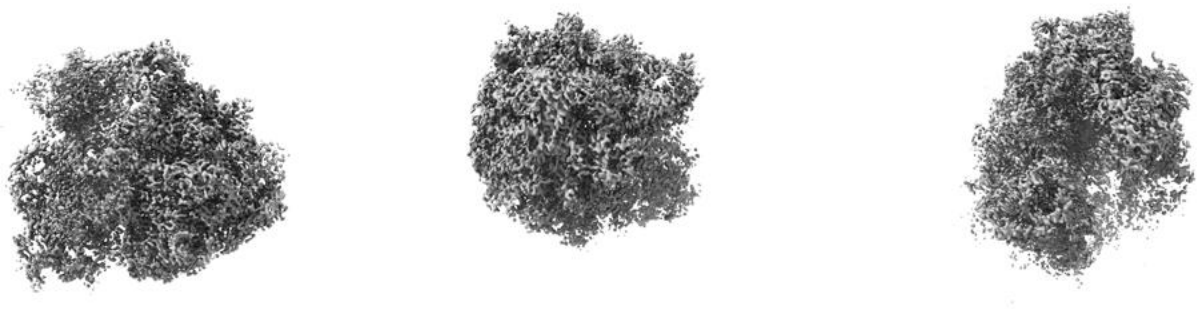


Z Index: 135

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

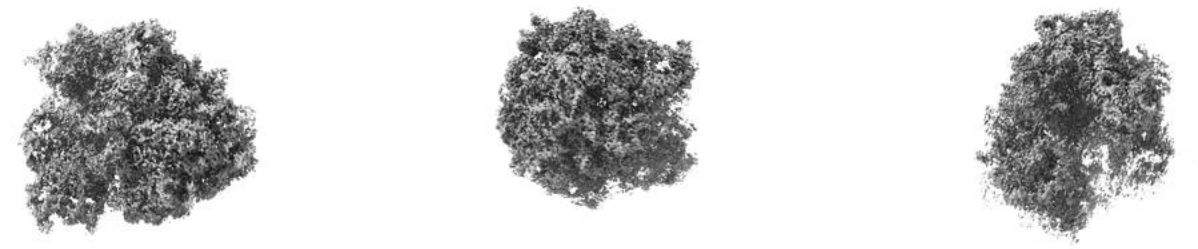
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

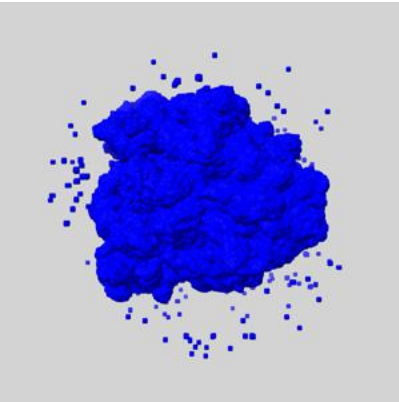
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

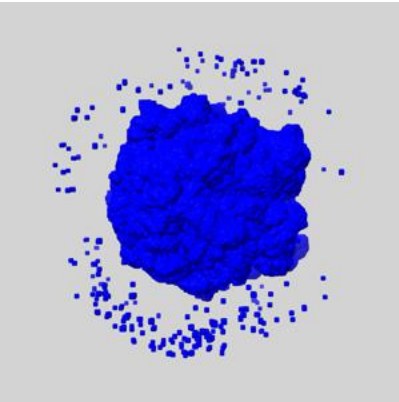
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

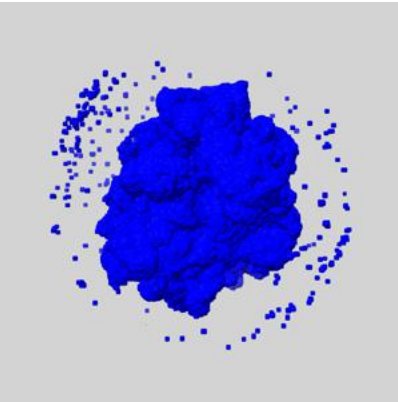
6.5.1 emd_13462_msk_1.map (i)



X



Y

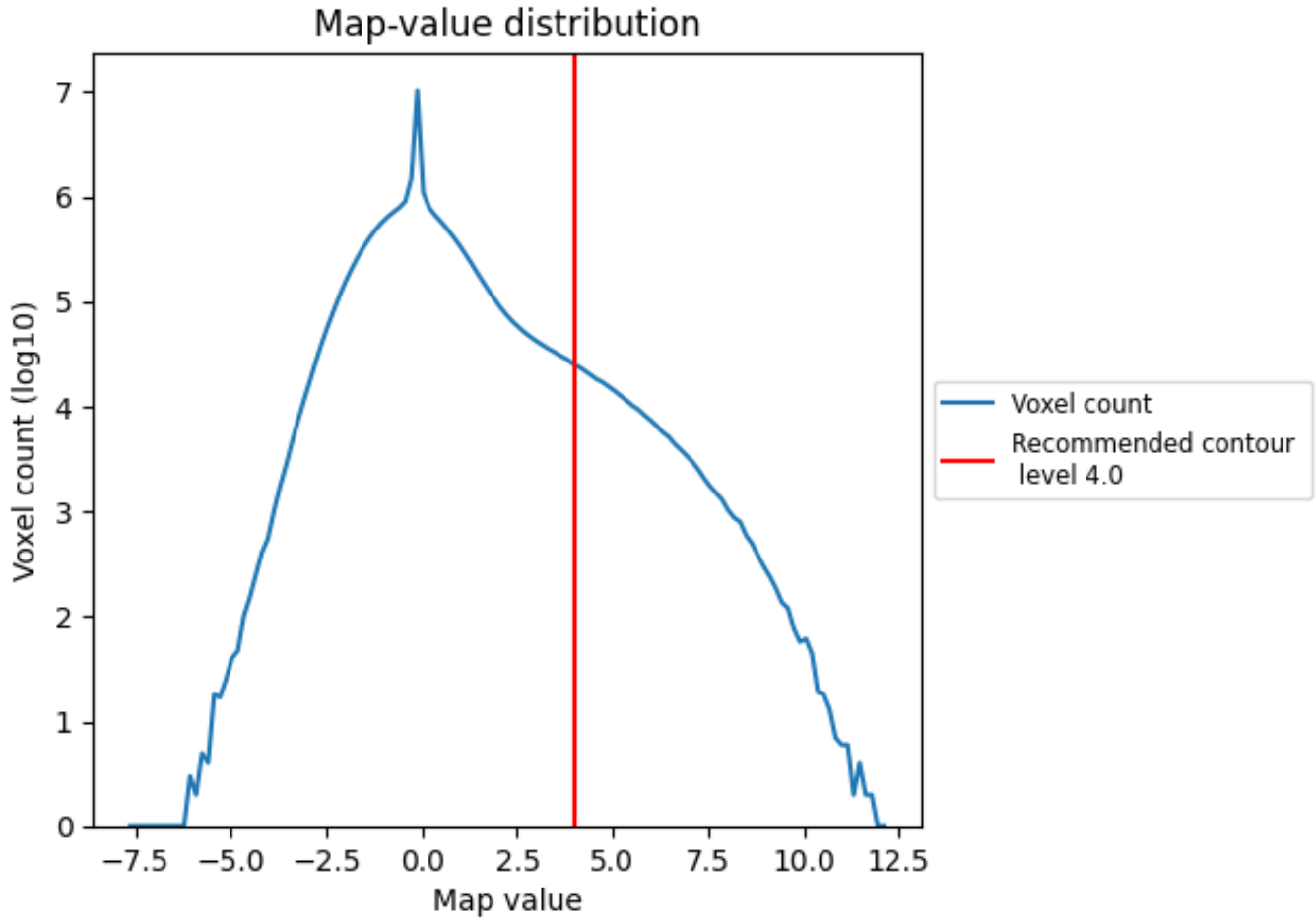


Z

7 Map analysis

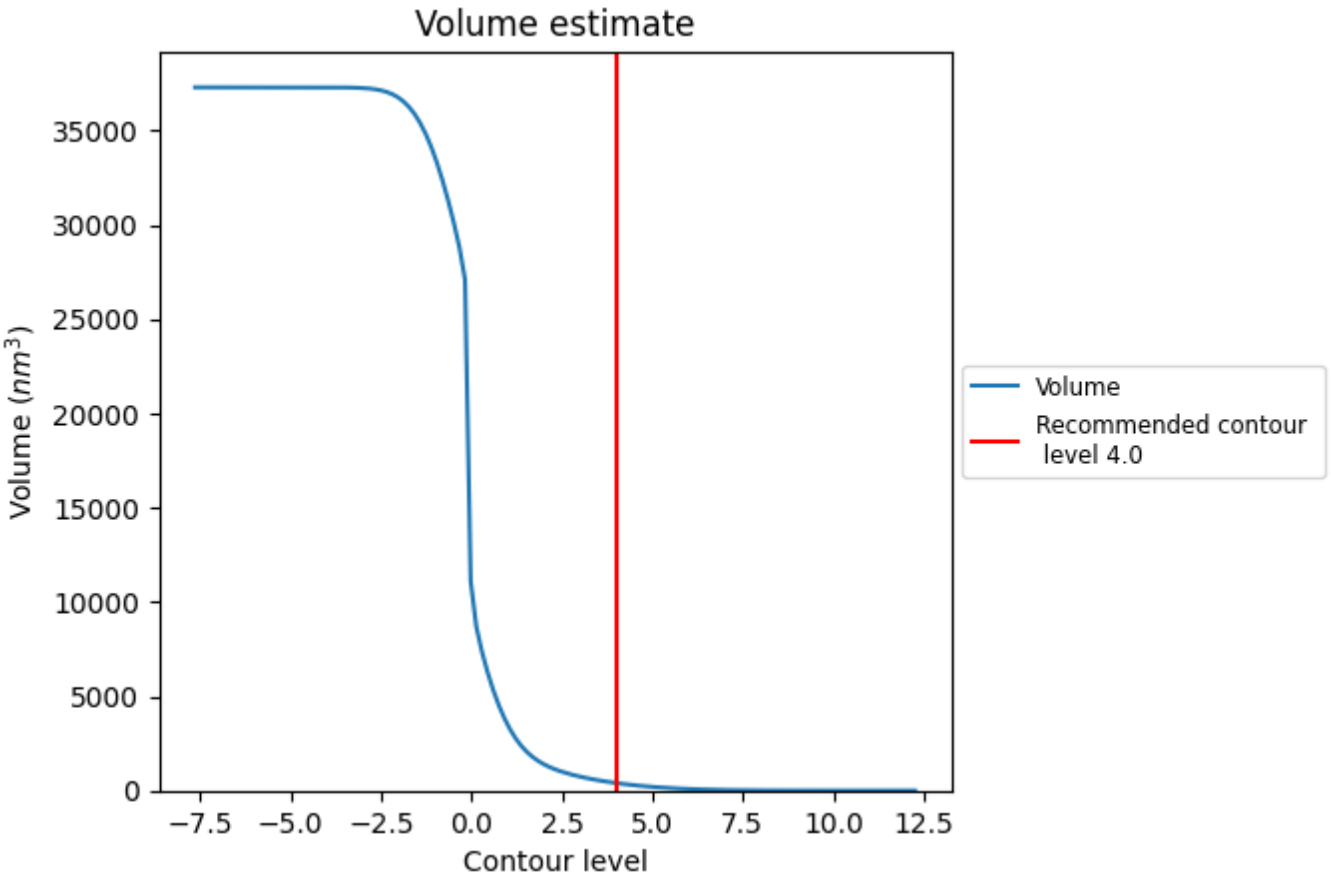
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

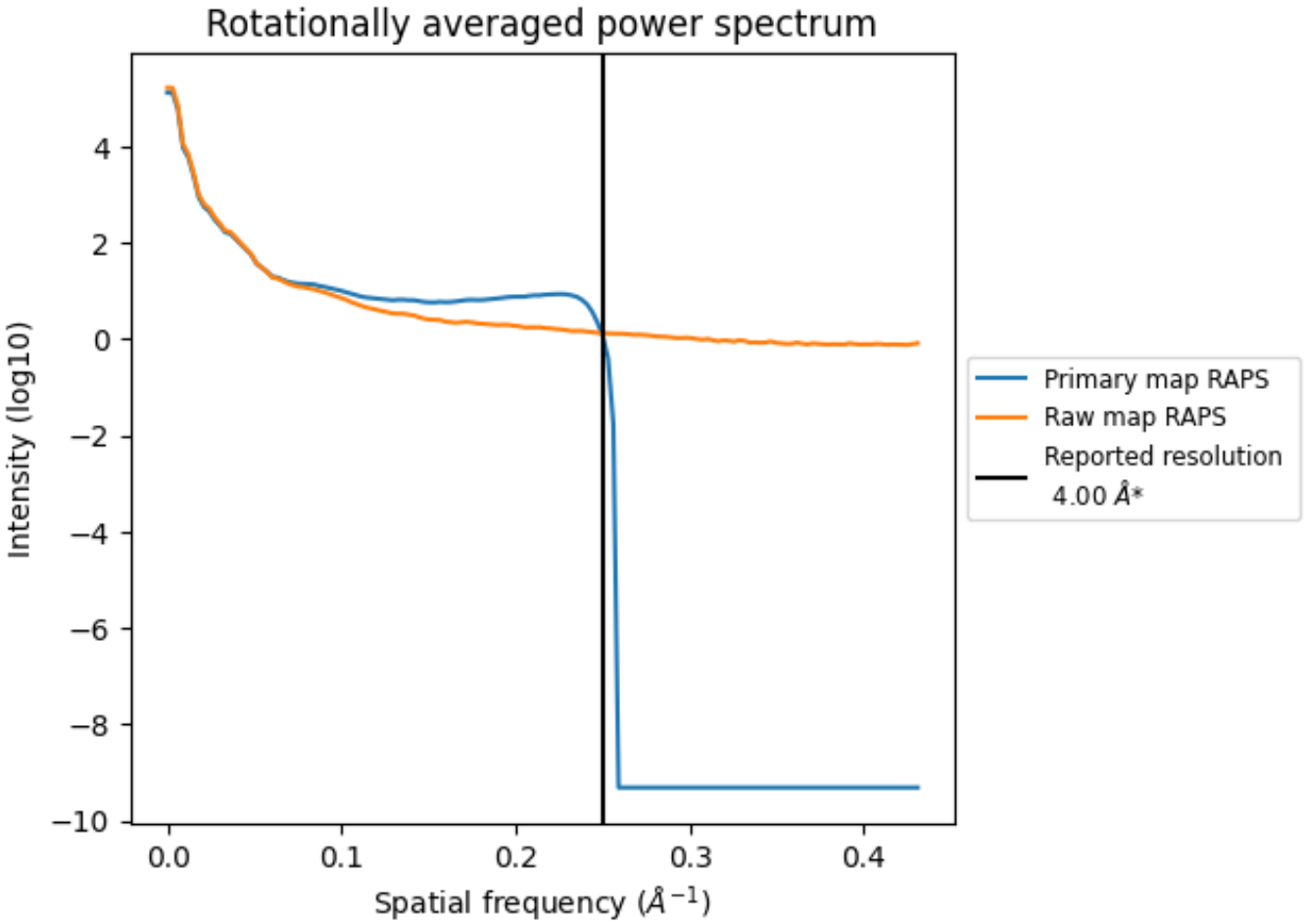
7.2 Volume estimate (i)



The volume at the recommended contour level is 397 nm^3; this corresponds to an approximate mass of 359 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

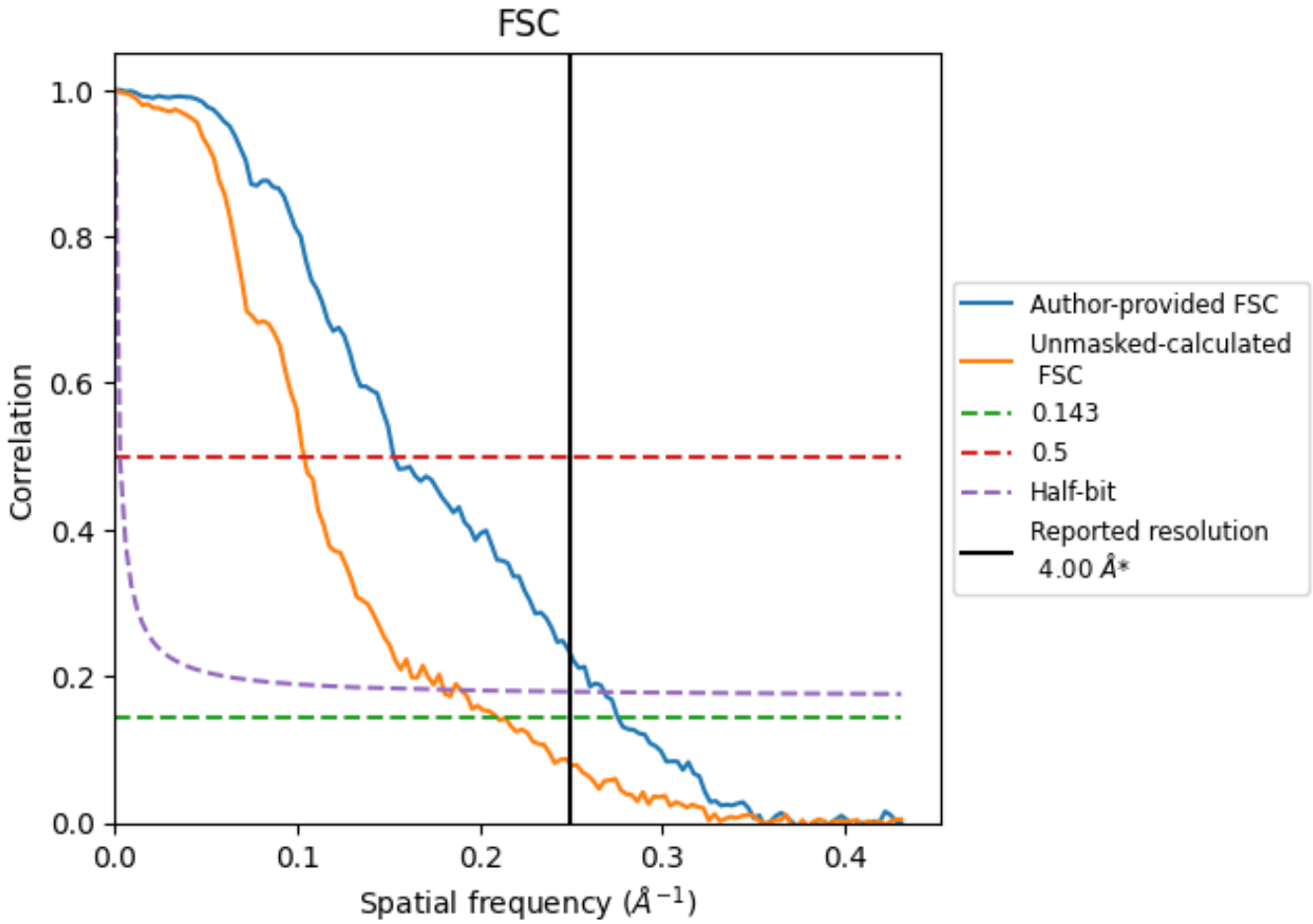


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

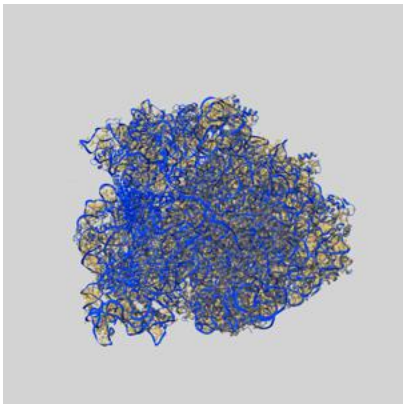
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.63	6.54	3.73
Unmasked-calculated*	4.77	9.64	5.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.77 differs from the reported value 4.0 by more than 10 %

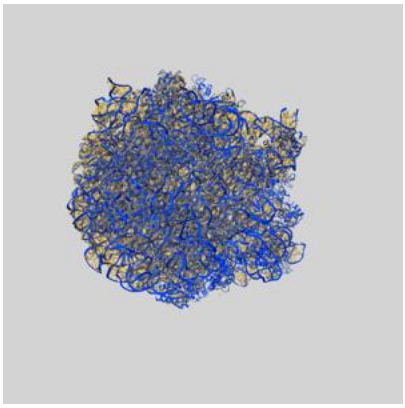
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13462 and PDB model 7PJW. Per-residue inclusion information can be found in section 3 on page 17.

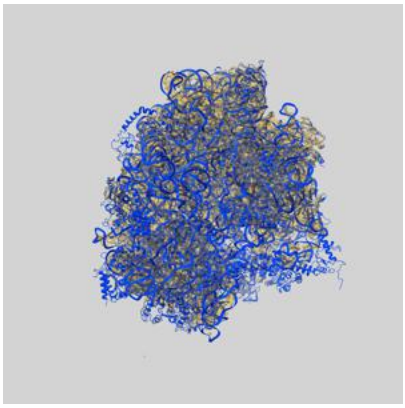
9.1 Map-model overlay



X



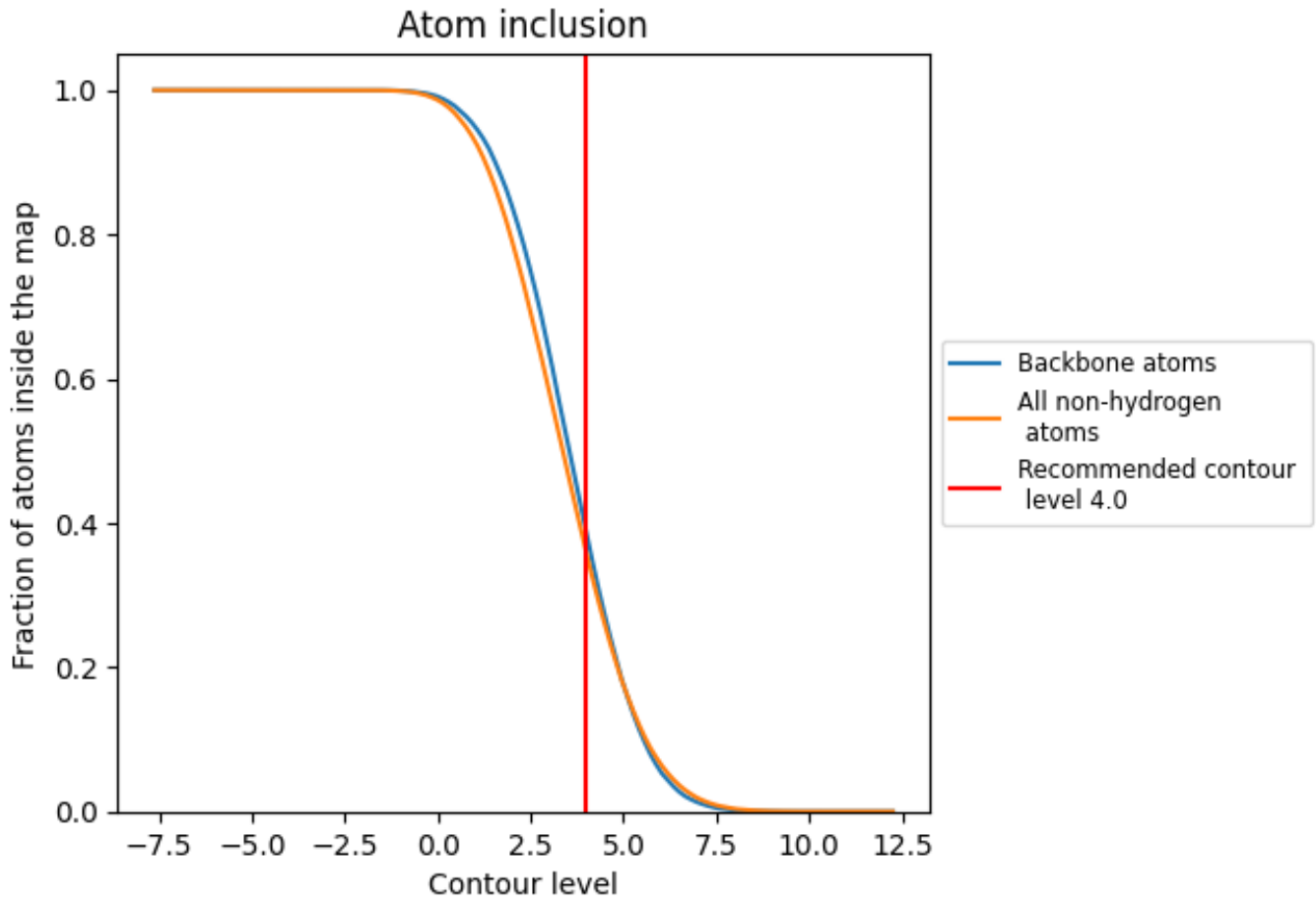
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 39% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.